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SCATTERING AND VARIATIONAL PRINCIPLES

by



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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies for acceptance, a thesis entitled SCATTERING AND VARIATIONAL PRINCIPLES, submitted by Parveen Nihal Singh Bawa, in partial fulfilment of the requirements for the degree of Master of Science.

ABSTRACT

A general review of the theory of scattering has been made. The formal theory of Lippmann and Schwinger and the explanation of nuclear reactions due to Bohr are discussed. To conclude, variational techniques of solving scattering problems are considered.

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INTRODUCTION

The process of scattering, thinking of the projectile and the target only, seems to be pretty simple. Extensive studies have been carried on both classically as well as quantum mechanically on this subject right from the beginning of this century. Many theoretical and experimental works have gone hand in hand in many areas of physics and chemistry.

In the beginning the main interest of study in physics was nuclear scattering. Faxen and Holtsmark⁴ introduced partial wave analysis for the first time and the first work on resonances was due to Debye.¹ Rutherford treated Coulomb scattering classically; the same results were obtained quantum mechanically later in the non-relativistic region. The conservation of flux was presented by Feenberg⁵ in 1932 in the form of optical theorem in quantum mechanics.

In general, the scattering problems cannot be solved exactly; either the method of successive approximations or the variational methods could be used. A great amount of work in the latter area was done by Hulthén,^{2a} Schwinger,^{4a} Kohn,^{1a} Kato,^{8a} Tamm^{3a} and others. From Schwinger's variational method the effective range theory was derived for the first time in connection with n-p and p-p scattering. Kohn^{12a} has developed the variational technique for scattering in momentum space.

For the formal theory of scattering, the S matrix was introduced by Wheeler⁶ and Heisenberg. A good, strictly mathematical treatment can be found in the article by Jauch.¹³ There are different formalisms for the S matrix, their equivalence has been shown by Fubini.⁹ In terms of the S operator Moses^{16a} has derived Kohn and Hulthén's variational principles. For formal theory of nuclear reactions, the R matrix, introduced by Wigner and Eisenbud is convenient to use. It does not assume any particular model to account for the observed reactions.

The most recent work on collision problems is the theory of dispersion relations, first given by Kronig³ and Kramers. The importance of dispersion relations lies in the fact that no detailed assumptions regarding the interaction are required. These relations have largely been used for the study of elementary particles.

In spite of such an extensive study on the subject of scattering there are many aspects which are yet to be explained. Furthermore, when it comes to their applications, some of the theoretical expressions are either not practical or, at least, very difficult to handle. The only simple formalism, easy to work with is elastic scattering at very low energies.

The above history shows how much work is needed to review the theory of scattering. In this thesis a general study of nuclear reactions, an introduction to

S matrix theory and a detailed study of variational principles have been made.

In Chapter I, the Lippmann-Schwinger theory of wave operators and the S matrix has been given. This particular formalism for S matrix was chosen because, later, the variational principle is applied to it. In Chapter II, nuclear reactions have been discussed very briefly. Partial wave analysis and detailed calculations have been omitted, only the important formulae and the physical concepts have been discussed. No R matrix treatment is included because it is not directly related to the Lippmann-Schwinger treatment of formal theory. Variational principles applied to scattering have been discussed extensively in Chapter III. Lastly, Chapter IV is devoted to some applications of variational principles.

All the references on scattering have not been included in the bibliography except for the very important ones. Also, there are three references, 3, 10, 2a which could not be obtained but are included for their historical importance. Up to 1951, Blatt and Weisskopf^{B1} gives a detailed list of publications. A latest very good list can be found in Scattering Theory of Waves and Particles by Newton.^{B7}

CHAPTER I

FORMAL THEORY OF SCATTERING

The process of scattering consists, essentially, of a beam of particles incident on the target and then scattered. In the remote past and in the remote future the particles are free, described by the free Hamiltonian H_0 . The dynamical properties of a quantum mechanical system are contained in the self adjoint, total energy operator H^0 on an abstract Hilbert space. In practice, for mathematical convenience, we take the incident beam as a plane wave. However, both physically and mathematically, this is not correct. Physically, the incident beam is never a plane wave, and mathematically, plane wave cannot be contained in a Hilbert space. The actual states, known as the eigenstates of H_0 , are represented by wave-packets which are elements of the Hilbert space.

The treatment given below is in the interaction picture. In the Schrödinger picture wave vectors depend on time while operators do not. The Schrödinger equation of motion gives the time dependence of the wave vectors. The Heisenberg equation of motion gives the time dependence of the operators and in this picture the state vectors are independent of time. This actually corresponds to the classical equation of motion for a dynamical variable. The

interaction picture is in between these. The time dependence of the state vectors is given by the Schrödinger equation involving the interaction Hamiltonian H_I only and the time dependence of the operators is given by Heisenberg's equation of motion involving only the free Hamiltonian H_0 .

The main object here is to find out the properties of the scattering operator which relates asymptotically free states in the past and the future. Scattering theory expresses this operator through the given interaction or vice versa. The procedure followed here is that due to Lippmann and Schwinger.⁷ Rigorous mathematical treatment of Hilbert space and functionals is not followed here. One can refer to the article by J.M. Jauch.¹³

a. Wave Operators

The time evolution of the state vectors in the interaction picture will be described in terms of the operators, $U_{\pm}(t)$, called the wave operators. Consider the two hermitian operators H_0 and H_I representing free particle and interaction Hamiltonians. The time dependent Schrödinger equation is

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = (H_0 + H_I) |\Psi(t)\rangle. \quad 1$$

To introduce the interaction picture, put

$$|\phi(t)\rangle = e^{+iH_0 \frac{t}{\hbar}} |\Psi(t)\rangle, \quad 2$$

then the state vectors in the interaction picture satisfy the equation

$$i\hbar \frac{\partial}{\partial t} |\phi(t)\rangle = H_I(t) |\phi(t)\rangle \quad 3$$

where

$$H_I(t) = e^{iH_0 \frac{t}{\hbar}} H_I e^{-iH_0 \frac{t}{\hbar}} \quad 4$$

is the interaction operator in the interaction picture.

The evolution of the states is expressed through the wave operators $U_{\pm}(t)$ i.e.

$$|\phi(t)\rangle = U_+(t) |\phi(-\infty)\rangle \quad 5a$$

$$|\phi(t)\rangle = U_-(t) |\phi(+\infty)\rangle. \quad 5b$$

The operator $U_+(t)$ is a solution of the equation

$$i\hbar \frac{\partial}{\partial t} U_+(t) = H_I(t) U_+(t) \quad 6a$$

with the boundary condition

$$U_+(-\infty) = 1. \quad 7a$$

With this boundary condition $U_+(t)$ has the integral representation

$$U_+(t) = 1 - \frac{i}{\hbar} \int_{-\infty}^t H_I(t') U_+(t') dt' \quad 8a$$

or

$$U_+(t) = 1 - \frac{i}{\hbar} \int_{-\infty}^{+\infty} \eta(t-t') H_I(t') U_+(t') dt' \quad 8b$$

where

$$\eta(\tau) = \begin{cases} 1 & \tau > 0 \\ 0 & \tau < 0 \end{cases} . \quad 9a$$

The analytic expression for $\eta(\tau)$ is

$$\begin{aligned} \eta(\tau) &= -\frac{1}{2\pi i} \int_{-\infty}^{+\infty} dk_0 \frac{1}{k_0 + i\varepsilon} e^{-ik_0 \tau} \\ &= \frac{1}{2\pi i} \int_{-\infty}^{+\infty} dk_0 \frac{1}{k_0 - i\varepsilon} e^{ik_0 \tau} , \end{aligned} \quad 9b$$

where ε is positive and the limit $\varepsilon \rightarrow +0$ is implied.

Similarly, $U_-(t)$ is the solution of the differential equation

$$i\hbar \frac{\partial}{\partial t} U_-(t) = H_I(t) U_-(t) \quad 6b$$

with the boundary condition

$$U_-(\infty) = 1 . \quad 7b$$

The integral representation is

$$U_-(t) = 1 + \frac{i}{\hbar} \int_t^{+\infty} H_I(t') U_-(t') dt' \quad 8c$$

or

$$U_-(t) = 1 + \frac{i}{\hbar} \int_{-\infty}^{+\infty} \eta(t'-t) H_I(t') U_-(t') dt' . \quad 8d$$

b. Scattering Matrix

Having defined the wave operators $U_{\pm}(t)$, the state vector $|\phi(+\infty)\rangle$ representing the entire system in its final

state corresponding to $t = \infty$ may be expressed as

$$|\phi(+\infty)\rangle = S |\phi(-\infty)\rangle \quad 10$$

namely ,

$$S = U_+(+\infty) \quad 11$$

is the scattering operator. From equations 5 and 11, one gets

$$U_+(t) = U_-(t) S . \quad 12$$

As $t \rightarrow -\infty$, equation 12 defines S^{-1} as

$$\begin{aligned} S^{-1} &= U_-(-\infty) \\ &= 1 + \frac{i}{\hbar} \int_{-\infty}^{+\infty} H_I(t) U_-(t) dt . \end{aligned} \quad 13$$

The probability that the system will be found eventually in a particular state with the initial state $|\phi_a\rangle$, is given by

$$\begin{aligned} W_{ba} &= |\langle \phi_b | S | \phi_a \rangle|^2 \\ &= |S_{ba}|^2 . \end{aligned} \quad 14$$

The eigenvalue equation for the free Hamiltonian is

$$(H_0 - E_a) |\phi_a\rangle = 0 . \quad 15$$

We demand that the eigenstates are normalised to unity i.e.

$$\langle \phi_a | \phi_b \rangle = \delta_{ab} \quad . \quad 16$$

Also we assume the closure relation

$$\sum_a |\phi_a\rangle \langle \phi_a| = 1 \quad . \quad 17$$

With the relations 16 and 17 and the unitarity of the S matrix (section 1f), the total scattering probability adds up to one.

For simplicity introduce the T operator defined by

$$T = S - 1 \quad . \quad 18$$

Using the unitarity of the S matrix (section 1f) we get from equation 18 the following relation

$$\begin{aligned} T^\dagger T &= (S^\dagger - 1)(S - 1) \\ &= S^\dagger S - S^\dagger - S + 1 \\ &= 1 - S^\dagger - (S - 1) \\ &= - (T + T^\dagger) \quad . \end{aligned} \quad 19$$

Equation 19 is important since the optical theorem will follow directly from it (section g). The scattering probability in terms of matrix elements of T can be written as

$$\begin{aligned} W_{ba} &= |\delta_{ba} + T_{ba}|^2 \\ W_{ba} &\stackrel{b \neq a}{=} |T_{ba}|^2 \quad . \end{aligned} \quad 20$$

It then follows from 8b and 11 that

$$\begin{aligned}
 T_{ba} &= -\frac{i}{\hbar} \int_{-\infty}^{+\infty} dt \langle \phi_b | H_I(t) U_+(t) | \phi_a \rangle \\
 &= -\frac{i}{\hbar} \int_{-\infty}^{+\infty} dt \langle \phi_b | e^{iH_0 \frac{t}{\hbar}} H_I e^{-iH_0 \frac{t}{\hbar}} U_+(t) | \phi_a \rangle \\
 &= -\frac{i}{\hbar} \int_{-\infty}^{+\infty} dt \langle \phi_b | H_I e^{i(E_b - H_0) \frac{t}{\hbar}} U_+(t) | \phi_a \rangle \\
 &= -\frac{i}{\hbar} \langle \phi_b | H_I | \psi_a^+(E_b) \rangle
 \end{aligned} \tag{21}$$

where

$$| \psi_a^+(E_b) \rangle = \int_{-\infty}^{+\infty} dt e^{i(E_b - H_0) \frac{t}{\hbar}} U_+(t) | \phi_a \rangle. \tag{22}$$

c. Lippmann-Schwinger Equation

The state $| \psi^+(E) \rangle$ will be given meaning in section

d. In order to find the simple integral equation satisfied by $| \psi^+(E) \rangle$ we proceed as follows: Substitute 8 in eq. 22, then

$$\begin{aligned}
 | \psi_a^+(E) \rangle &= \int_{-\infty}^{+\infty} dt e^{i(E - H_0) \frac{t}{\hbar}} | \phi_a \rangle - \\
 &\quad \frac{i}{\hbar} \int_{-\infty}^{+\infty} dt \int_{-\infty}^{+\infty} dt' \eta(t - t') e^{i(E - H_0) \frac{t}{\hbar}} H_I(t') U_+(t') | \phi_a \rangle.
 \end{aligned}$$

Using the eigenvalue equation 15, this simplifies to

$$\begin{aligned}
|\psi_a^+(E)\rangle &= 2\pi\hbar\delta(E-E_a)|\phi_a\rangle - \frac{i}{\hbar} \int_{-\infty}^{+\infty} dt \int_{-\infty}^{+\infty} dt' \eta(t-t') e^{\frac{i(E-H_0)t}{\hbar}} \\
&\quad \times e^{\frac{iH_0 t'}{\hbar}} e^{-\frac{iEt'}{\hbar}} e^{\frac{iEt'}{\hbar}} H_I e^{-\frac{iH_0 t'}{\hbar}} U_+(t') |\phi_a\rangle \\
&= 2\pi\hbar\delta(E-E_a)|\phi_a\rangle - \frac{i}{\hbar} \int_{-\infty}^{+\infty} dt \int_{-\infty}^{+\infty} dt' \eta(t-t') \\
&\quad \times e^{\frac{i(E-H_0)(t-t')}{\hbar}} H_I e^{\frac{i(E-H_0)t'}{\hbar}} U_+(t') |\phi_a\rangle .
\end{aligned}$$

Put $t-t'=\tau$, then $dt dt' = d\tau dt'$ and we get

$$\begin{aligned}
|\psi_a^+(E)\rangle &= 2\pi\hbar\delta(E-E_a)|\phi_a\rangle - \frac{i}{\hbar} \int_{-\infty}^{+\infty} d\tau \int_{-\infty}^{+\infty} dt' \eta(\tau) e^{\frac{i(E-H_0)\tau}{\hbar}} H_I \\
&\quad \times e^{\frac{i(E-H_0)t'}{\hbar}} U_+(t') |\phi_a\rangle \\
&= 2\pi\hbar\delta(E-E_a)|\phi_a\rangle - \frac{i}{\hbar} \int_{-\infty}^{+\infty} dt' \int_0^{\infty} d\tau e^{\frac{i(E-H_0)\tau}{\hbar}} H_I \\
&\quad \times e^{\frac{i(E-H_0)t'}{\hbar}} U_+(t') |\phi_a\rangle
\end{aligned}$$

$$|\psi_a^+(E)\rangle = 2\pi\hbar\delta(E-E_a)|\phi_a\rangle + \frac{1}{E-H_0+i\epsilon} H_I |\psi_a^+(E)\rangle \quad 23a$$

where (after introducing the integrating factor)

$$- \frac{i}{\hbar} \int_0^{\infty} d\tau e^{\frac{i(E-H_0)\tau}{\hbar}} e^{-\epsilon \frac{|\tau|}{\hbar}} = \frac{1}{E-H_0+i\epsilon} .$$

If we put

$$|\psi_a^+(E)\rangle = 2\pi\hbar\delta(E-E_a)|\psi_a^+\rangle , \quad 24$$

then

$$2\pi\hbar\delta(E-E_a)|\psi_a^+\rangle = 2\pi\hbar\delta(E-E_a)|\phi_a\rangle + \frac{1}{E-H_0+i\epsilon} 2\pi\hbar\delta(E-E_a)H_I|\psi_a^+\rangle.$$

By integrating over E we obtain

$$|\psi_a^+\rangle = |\phi_a\rangle + \frac{1}{E_a-H_0+i\epsilon} H_I|\psi_a^+\rangle \quad 23b$$

which is the Lippmann Schwinger equation. The positive sign of ϵ indicates an outgoing scattered wave (Chapter I h).

Sometimes we shall have to use a negative sign such that

$$|\psi_a^-\rangle = |\phi_a\rangle + \frac{1}{E-H_0-i\epsilon} H_I|\psi_a^-\rangle \quad 23c$$

with

$$|\psi_a^-(E)\rangle = \int_{-\infty}^{+\infty} dt e^{i(E-H_0)\frac{t}{\hbar}} U_-(t)|\phi_a\rangle.$$

Equations 24a and 24b can be written down in a new notation as

$$|\psi_a^\pm\rangle = |\phi_a\rangle + G_\pm(E_a) H_I|\psi_a^\pm\rangle \quad 25$$

where

$$G_\pm(E_a) = \lim_{\epsilon \rightarrow 0} \frac{1}{E_a-H_0 \pm i\epsilon} \quad 26$$

is the Green's function for the homogeneous equation

$$(H_0 - E)|\phi_a\rangle = 0.$$

These equations provide a time independent formulation of scattering and the small $i\epsilon$ automatically selects the outgoing and the incoming spherical waves as will be shown in section h of Chapter I.

d. The Scattering State

The state $|\phi_a\rangle$ is known to be an eigenstate of the free Hamiltonian. Now we give meaning to the state $|\psi_a^+\rangle$. Multiply equation 23 by $(E-H_0+i\epsilon)$ and let $\epsilon \rightarrow 0$, we get

$$\begin{aligned}(E-H_0)|\psi_a^+(E)\rangle &= 2\pi\hbar(E-H_0)\delta(E-E_a)|\phi_a\rangle + H_I|\psi_a^+(E)\rangle \\ &= 2\pi\hbar(E-E_a)\delta(E-E_a)|\phi_a\rangle + H_I|\psi_a^+(E)\rangle.\end{aligned}$$

Since the first term on the R.H.S. is zero, it simplifies to

$$(E-H_0-H_I)|\psi_a^+(E)\rangle = 0$$

or

$$(E-H)|\psi_a^+(E)\rangle = 0 \tag{27}$$

where H is the total Hamiltonian. Thus equation 27 shows that $|\psi_a^+(E)\rangle$ ($|\psi_a^-(E)\rangle$) is an eigenstate of the total Hamiltonian and is known as the scattering state of the system. It has been assumed that the bound states appear only for $E < 0$ and scattering states for $E > 0$ so that the two lie in orthogonal spaces.

Equation 25 can be written in terms of H instead of H_0 . Multiply eq. 25 by $(E-H_0 \pm i\epsilon)$, it gives

$$(E-H_0 \pm i\epsilon) |\psi_a^\pm\rangle = (E-H_0 \pm i\epsilon) |\phi_a\rangle + H_I |\psi_a^\pm\rangle$$

$$(E-H \pm i\epsilon) |\psi_a^\pm\rangle = (E-H_0 - H_I \pm i\epsilon) |\phi_a\rangle + H_I |\phi_a\rangle$$

$$(E-H \pm i\epsilon) |\psi_a^\pm\rangle = (E-H \pm i\epsilon) |\phi_a\rangle + H_I |\phi_a\rangle \quad .$$

Hence

$$|\psi_a^\pm\rangle = |\phi_a\rangle + \frac{1}{E-H \pm i\epsilon} H_I |\phi_a\rangle. \quad 28$$

This equation is useful in multiple scattering theory.^{B3}

e. Reaction Matrix

In order to make the unitarity of the S matrix somewhat more manifest, we introduce another matrix K , following Lippmann and Schwinger, which is called the reaction matrix.

For this purpose we consider the new operator defined by

$$V(t) = U_+(t) \frac{2}{1+S} = U_-(t) \frac{2}{1+S^{-1}} \quad . \quad 29$$

The two equivalent expressions in eq. 29 follow from eq.12 and unitarity of the S matrix; i.e.

$$\frac{2U_+(t)}{1+S} = \frac{2U_-(t)S}{1+S} = \frac{2U_-(t)}{1+S^{-1}} \quad .$$

It follows from equations 7 and 11 that

$$V(-\infty) = \frac{2}{1+S} \quad 30a$$

$$V(+\infty) = \frac{2S}{1+S} \quad 30b$$

and hence

$$\frac{1}{2} [V(\infty) + V(-\infty)] = 1 \quad 31$$

From equations 30a, 7b and 29 we get

$$V(\infty) = V^\dagger(-\infty) \quad 32$$

These conditions lead to the definition of the reaction matrix K with

$$V(\infty) = 1 - \frac{1}{2} iK$$

$$V(-\infty) = 1 + \frac{1}{2} iK.$$

Equation 32 gives

$$K^\dagger = K.$$

From equation 30

$$S = \frac{V(\infty)}{V(-\infty)} = \frac{1 - \frac{1}{2} iK}{1 + \frac{1}{2} iK} \quad 33$$

The unitarity of the S matrix follows immediately from the above expression.⁷

Substituting eqs. 8 in eq. 29 and using the expression 30 we get

$$V(t) = V(-\infty) - \frac{i}{\hbar} \int_{-\infty}^t H_I(t') V(t') dt'$$

$$V(t) = V(\infty) + \frac{i}{\hbar} \int_t^{\infty} H_I(t') V(t') dt'$$

which can together be written as

$$V(t) = 1 - \frac{i}{2\hbar} \int_{-\infty}^{+\infty} \epsilon(t-t') H_I(t') V(t') dt' \quad 34$$

where

$$\epsilon(t-t') = \begin{cases} 1 & t' < t \\ -1 & t' > t \end{cases} .$$

The operator $V(t)$ clearly shows the symmetry between past and future.

Finally the reaction matrix gets the form

$$K = \frac{1}{\hbar} \int_{-\infty}^{+\infty} H_I(t) V(t) dt . \quad 35$$

From equations 18 and 33 we obtain

$$T = S - 1 = \frac{-iK}{1 + \frac{1}{2} iK}$$

or

$$T + \frac{1}{2} iKT = -iK \quad 36$$

which is Heitler's damping equation (B3, Chap. V). Equation 33 shows that

$$SK = KS \quad 37$$

and therefore K commutes with T also. There is a direct relationship between the eigenstates of S , K and T operators.^{B13} For describing many of the physical processes it is more convenient to use K and T rather than the S operator.

f. Unitarity of the Wave Operators and the S Matrix

Before investigating the unitarity of S matrix, the unitarity of the wave operators $U_{\pm}(t)$ will be checked. Certain properties of $U_{\pm}(t)$ will be derived which are later applied to prove the unitarity of S .

Consider equation 22 which can be written as

$$2\pi\hbar\delta(E-E_a)|\psi_a^+\rangle = \int_{-\infty}^{+\infty} dt' e^{i(E-H_0)\frac{t'}{\hbar}} e^{-\epsilon\frac{|t'|}{\hbar}} U_+(t')|\phi_a\rangle .$$

Integrating over E from $-\infty$ to $+\infty$, we obtain

$$|\psi_a^+\rangle = U_+(0)|\phi_a\rangle . \quad 38$$

From equations 38 and closure relation 17, the following two relations are obtained

$$U_+(0) = \sum_a |\psi_a^+\rangle \langle \phi_a| \quad 39a$$

$$U_+^\dagger(0) = \sum_a |\phi_a\rangle \langle \psi_a^+| . \quad 39b$$

Relations 39a,b give

$$\begin{aligned}
U_+^\dagger(0)U_+(0) &= \sum_a |\phi_a\rangle\langle\psi_a^+| \psi_a^+\rangle\langle\phi_a| \\
&= \sum_a |\phi_a\rangle\langle\phi_a| \\
&= 1
\end{aligned}
\tag{40}$$

$$U_+(0)U_+^\dagger(0) = \sum_a |\psi_a^+\rangle\langle\psi_a^+| \quad . \tag{41}$$

The scattering states do not in general form a complete set because if a bound state exists it cannot be expressed as a linear combination of the scattering states. The scattering states and the bound states $|\psi_B\rangle$ together form a complete set, i.e.

$$\sum_a |\psi_a\rangle\langle\psi_a| + \sum_B |\psi_B\rangle\langle\psi_B| = 1 \quad . \tag{42}$$

Therefore, if the bound states exist, then

$$U_+(0)U_+^\dagger(0) = 1 - \sum_B |\psi_B\rangle\langle\psi_B| \quad . \tag{43}$$

The second term on the R.H.S. is called the unitary deficiency.¹³ On the same lines we have the relation

$$U_-(0) = \sum_a |\psi_a^-\rangle\langle\phi_a| \tag{44a}$$

$$U_-^\dagger(0) = \sum_a |\phi_a\rangle\langle\psi_a^-| \quad . \tag{44b}$$

These relations give

$$U_-^\dagger(0)U_-(0) = 1 \tag{45}$$

and

$$U_{-}(0)U_{-}^{\dagger}(0) = 1 - \sum_B |\psi_B\rangle\langle\psi_B| . \quad 46$$

Hence we conclude that the wave operators $U_{\pm}(t)$ are not unitary in general.

Here we introduce a small change in the notation to prove certain properties of $U_{\pm}(t)$ which are to be used later. Put

$$U_{+}(t) \equiv U(t, -\infty) \quad 47a$$

$$U_{-}(t) \equiv U(t, +\infty) . \quad 47b$$

In this new notation, consider the operator $U(t, t')$ which evolves the state $|\phi(t)\rangle$ from $|\phi(t')\rangle$, then

$$\begin{aligned} |\phi(t)\rangle &= U(t, t') |\phi(t')\rangle \\ &= U(t, t') U(t', t_0) |\phi(t_0)\rangle \\ &= U(t, t_0) |\phi(t_0)\rangle . \end{aligned}$$

Again, using the completeness relation we get

$$U(t, t_0) = U(t, t') U(t', t_0) . \quad 48$$

Multiply equation 45 from the right by $U(\infty, 0)$, then with $U(t, t) = 1$ we get

$$U^{\dagger}(0, \infty) = U(\infty, 0) \quad 49$$

and therefore

$$U(\infty, 0) = \sum_a |\phi_a\rangle\langle\psi_a^-| \quad . \quad 50$$

Physically $U(0, -\infty)$ describes the switching on process from non-interacting particle to interacting particle, while $U(\infty, 0)$ describes the switching off process.

The unitarity of S follows from the fact that the bound states are orthogonal to the scattering states. Using equations 11, 43, 48 and 50 we get

$$\begin{aligned} SS^\dagger &= U(\infty, -\infty)U^\dagger(\infty, -\infty) \\ &= U(\infty, 0)U(0, -\infty)U^\dagger(0, -\infty)U^\dagger(\infty, 0) \\ &= \sum_a |\phi_a\rangle\langle\psi_a^-| \left(1 - \sum_B |\psi_B\rangle\langle\psi_B|\right) \sum_b |\psi_b^- \rangle\langle\phi_b| \\ &= \sum_a |\phi_a\rangle\langle\phi_a| \\ &= 1 \quad . \end{aligned} \quad 51$$

Also from 11, 40 and 48

$$\begin{aligned} S^\dagger S &= U^\dagger(\infty, -\infty)U(\infty, -\infty) \\ &= U^\dagger(0, -\infty)U^\dagger(\infty, 0)U(\infty, 0)U(0, -\infty) \\ &= U^\dagger(0, -\infty)U^\dagger(\infty, 0)U^\dagger(0, \infty)U(0, -\infty) \\ &= U^\dagger(0, -\infty)U(0, -\infty) \\ &= 1 \quad . \end{aligned} \quad 52$$

Relations 51 and 52 together prove the unitarity of the S

matrix. Physically it implies the conservation of probability.

Matrix elements of S can also be written as follows:

$$\begin{aligned}\langle \phi_b | S | \phi_a \rangle &= \langle \phi_b | U(\infty, 0) U(0, -\infty) | \phi_a \rangle \\ &= \sum_c \sum_d \langle \phi_b | \phi_c \rangle \langle \psi_c^- | \psi_d^+ \rangle \langle \phi_d | \phi_a \rangle .\end{aligned}$$

Due to the orthonormality relation

$$S_{ba} = \langle \psi_b^- | \psi_a^+ \rangle . \quad 53$$

Thus we have expressed the matrix elements of S in terms of the scattering states.

g. Scattering Cross Section and Optical Theorem

The most important expression in the theory of scattering is for the scattering cross section, which is an experimentally measurable quantity. For this we have to derive an expression for the transition probability.

With the help of eq. 24, T_{ba} in eq. 21 can be written as

$$T_{ba} = -2\pi i \delta(E_b - E_a) T_{ba} \quad 54$$

where

$$T_{ba} = \langle \phi_b | H_I | \psi_a^+ \rangle . \quad 55$$

The transition probability from the state $|\phi_a\rangle$ to the state $|\phi_b\rangle$ is given by

$$\begin{aligned}
 W_{ba} &= |T_{ba}|^2 & b \neq a \\
 &= 4\pi^2 \{\delta(E_b - E_a)\}^2 |T_{ba}|^2 \\
 &= \frac{2\pi}{\hbar} \delta(E_b - E_a) |T_{ba}|^2 \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{+\infty} e^{i(E_b - E_a)\frac{t}{\hbar} - \epsilon \frac{|t|}{\hbar}} dt \\
 &= \frac{2\pi}{\hbar} \delta(E_a - E_b) |T_{ba}|^2 \int_{-\infty}^{+\infty} dt .
 \end{aligned} \tag{56}$$

This states that the transition occurs only between states of equal energy for the separated system and with intensity proportional to the total time of effective interaction. As $\epsilon \rightarrow 0$, the latter becomes infinitely large. The transition probability per unit time from the state $|\phi_a\rangle$ to the state $|\phi_b\rangle$ is, therefore

$$\omega_{ba} = \frac{2\pi}{\hbar} \delta(E_b - E_a) |T_{ba}|^2 . \tag{57}$$

The scattering cross section is defined by

$$\sigma_{ba} = \frac{\omega_{ba}}{\text{incident flux}} .$$

If V is the volume in which the state vectors have been normalised and v_{rel} is the relative velocity, then

$$\sigma_{ba} = \frac{V}{v_{\text{rel}}} \omega_{ba} . \tag{58}$$

The unitarity of S has been used in equation 19 from which the optical theorem will be derived. From equation 19 we get

$$(T^\dagger T)_{ba} = - (T_{ba} + T_{ba}^\dagger)$$

or

$$\sum_c T_{cb}^* T_{ca} = - (T_{ba} + T_{ab}^*) . \quad 59$$

Substitute eq. 54 in eq. 59, to give

$$-2\pi i \sum_c \delta(E_c - E_b) \delta(E_c - E_a) T_{cb}^* T_{ca} = \delta(E_a - E_b) [T_{ba} - T_{ab}^*] .$$

Removing one δ -function we get the simplified expression in the forward direction

$$\pi \sum_c \delta(E_c - E_a) |T_{ca}|^2 = - \text{Im } T_{aa} \quad (E_a = E_b) .$$

In terms of the transition probability it becomes

$$\text{Im } T_{aa} = - \frac{\hbar}{2} \sum_{c \neq a} \omega_{ca} - \pi \delta(E_c - E_a) |T_{aa}|^2 .$$

The second term on the R.H.S. is the transition probability in the forward direction. The transition probability is proportional to the density of final states. For just one state $c=a$, when the integration is carried over the solid angle $d\Omega$ pointing in the direction $\theta=0$, the contribution is zero; therefore, we can write the above expression as

$$\text{Im } T_{aa} = -\frac{\hbar}{2} \sum_c \omega_{ca} \quad . \quad 60$$

In terms of the scattering cross section eq. 60, with the help of eq. 58, takes the form

$$\text{Im } T_{aa} = -\frac{\hbar}{2} \frac{v_{\text{rel}}}{V} \sigma_T \quad . \quad 61$$

Equation 61 is the optical theorem which relates the forward scattering amplitude to the total scattering cross section. It states that the flux taken away from the incident or the forward direction contributes to the total flux scattered; and hence it states the law of conservation of flux. It is clear that the optical theorem is derived from the unitary property of the S matrix (eq. 19) and therefore unitarity of the S matrix also implies the conservation of flux. We have already shown that with the normalisation condition (eq. 16), closure relation (eq.17) and the unitarity of S the total scattering probability adds up to unity.

It may be mentioned here that this formalism is not only important for scattering but for decay systems in general. For example, it is useful in determining the lifetimes^{B11} and decay rates.

h. Scattering by a Central Potential

In order to relate these formulae to the ordinary quantum mechanical scattering, consider the scattering of

a scalar particle with momentum k by a central potential $V(r) = H_I$. Then the Lippmann-Schwinger equation in coordinate representation is written as

$$\begin{aligned} \langle \vec{r} | \psi_a^\pm \rangle &= \langle \vec{r} | \phi_a \rangle + \iint \langle \vec{r} | \frac{1}{E - H_0 \pm i\epsilon} | \vec{r}' \rangle \langle \vec{r}' | V | \vec{r}'' \rangle \langle \vec{r}'' | \psi_a^\pm \rangle d\vec{r}' d\vec{r}'' \\ \psi_a^\pm(\vec{r}) &= \phi_a(\vec{r}) + \frac{1}{E + \frac{\nabla^2}{2m} \pm i\epsilon} \int V(\vec{r}'') \psi_a^\pm(\vec{r}'') \delta(\vec{r} - \vec{r}'') d\vec{r}'' \\ &= \phi_a(\vec{r}) + \frac{1}{E + \frac{\nabla^2}{2m} \pm i\epsilon} \frac{1}{(2\pi)^3} \iint V(r'') \psi_a^\pm(\vec{r}'') e^{i\vec{k}' \cdot (\vec{r} - \vec{r}'')} \\ &\quad \times d\vec{r}'' d\vec{k}' \quad . \quad 62 \end{aligned}$$

The eigenfunction of the free Hamiltonian is $e^{i\vec{k} \cdot \vec{r}}$ which represents the incident plane wave. Therefore

$$\frac{1}{E - \frac{\nabla^2}{2m} \pm i\epsilon} e^{i\vec{k}' \cdot \vec{r}} = \frac{2m}{\hbar^2} \frac{e^{i\vec{k}' \cdot \vec{r}}}{k^2 - k'^2 \pm i\epsilon} \quad . \quad 63$$

With the help of eq. 63, eq. 62 can be written as

$$\psi^\pm(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} + \frac{2m}{\hbar^2 (2\pi)^3} \iint V(r') \psi^\pm(\vec{r}') \frac{e^{i\vec{k}' \cdot (\vec{r} - \vec{r}')}}{k^2 - k'^2 \pm i\epsilon} d\vec{r}' d\vec{k}' \quad . \quad 64$$

In brief notation eq. 64 is written as

$$\psi^\pm(\vec{r}) = \phi(\vec{r}) + \int G^\pm(\vec{r}, \vec{r}') U(r') \psi(\vec{r}') d\vec{r}' \quad 65$$

where

$$U(r) = \frac{2m}{\hbar^2} V(r)$$

and

$$G^{\pm}(\vec{r}, \vec{r}') = \frac{1}{(2\pi)^3} \int \frac{e^{i\vec{k}' \cdot (\vec{r} - \vec{r}')}}{k^2 - k'^2 \pm i\epsilon} d\vec{k}' \quad 66$$

is the Green's function, which satisfies the equation

$$(\nabla^2 + k^2)G^{\pm}(\vec{r}, \vec{r}') = + \delta(\vec{r} - \vec{r}') . \quad 67$$

To evaluate $G^{\pm}(\vec{r}, \vec{r}')$, put $\rho = |\vec{r} - \vec{r}'|$. Consider only $G^+(\vec{r}, \vec{r}')$, first for which, we have introduced $+i\epsilon$ in the denominator. Applying Cauchy's integral theorem we get

$$\begin{aligned} G^+(\vec{r}, \vec{r}') &= - \frac{2\pi}{i\rho(2\pi)^3} \int_0^{\infty} \frac{(e^{ik'\rho} - e^{-ik'\rho})k' dk'}{[k' - (k + \frac{i\epsilon}{2k})][k' + (k + \frac{i\epsilon}{2k})]} \\ &= - \frac{1}{2 \cdot (2\pi)^2 i\rho} \cdot 2\pi i e^{ik\rho} . \end{aligned}$$

The limit $\epsilon \rightarrow +0$ is implied. Thus the simplified expression for $G^+(\vec{r}, \vec{r}')$ is

$$G^+(\vec{r}, \vec{r}') = - \frac{1}{4\pi} \frac{e^{ik|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|} . \quad 68a$$

Physically, it represents an outgoing spherical wave.

Similarly, introducing $-i\epsilon$ in the denominator, we get the expression for $G^-(\vec{r}, \vec{r}')$:

$$\begin{aligned}
G^-(\vec{r}, \vec{r}') &= \frac{1}{(2\pi)^3} \int \frac{e^{i\vec{k}' \cdot |\vec{r} - \vec{r}'|}}{k^2 - k'^2 - i\epsilon} d\vec{k}' \\
&= -\frac{1}{4\pi} \frac{e^{-ik|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|} .
\end{aligned} \tag{68b}$$

This represents an incoming spherical wave. With the help of eq. 68a,b, 65 can be written down as

$$\psi^\pm(\vec{r}) = e^{ikz} - \frac{1}{4\pi} \int \frac{e^{\pm ik|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|} U(r') \psi^\pm(\vec{r}') d\vec{r}' . \tag{69}$$

In scattering, we are concerned with the asymptotic states, consequently we have $r \gg r'$ and therefore

$$|\vec{r} - \vec{r}'| \approx r - r' \cos\theta , \quad \frac{1}{|\vec{r} - \vec{r}'|} \sim \frac{1}{r}$$

where θ is the angle between \vec{r} and \vec{r}' ; and \vec{k}' is the propagation vector for the scattered wave. With this approximation, $\psi^+(\vec{r})$ in eq. 69 becomes

$$\psi^+(\vec{r}) \rightarrow e^{ikz} - \frac{e^{ikr}}{4\pi r} \int e^{-i\vec{k}' \cdot \vec{r}'} U(r') \psi^+(\vec{r}') d\vec{r}' . \tag{70}$$

Put

$$f(\theta) = -\frac{1}{4\pi} \int e^{-i\vec{k}' \cdot \vec{r}'} U(r') \psi^+(\vec{r}') d\vec{r}' . \tag{71}$$

Then the asymptotic form of the solution of the Lippmann-Schwinger equation in the co-ordinate representation is

$$\psi^+(\vec{r}) \approx e^{ikz} + f(\theta) \frac{e^{ikr}}{r} . \tag{72}$$

Thus $f(\theta)$ is the scattering amplitude. In general, it will depend on the azimuthal angle ϕ also if the incident wave does not possess the cylindrical symmetry. Equation 72 is the familiar expression for the wave description of scattering in centre of mass system.

To write down the optical theorem (eq. 61) in co-ordinate representation, we have to determine the T matrix elements. Following the same procedure as for eq. 62, we get from equation 55

$$\begin{aligned} T_{ba} &= \iint \langle \phi_b | \vec{r} \rangle \langle \vec{r} | V | \vec{r}' \rangle \langle \vec{r}' | \psi^\pm \rangle d\vec{r}' d\vec{r} \\ &= \iint \phi_b^*(\vec{r}) V(r) \delta(\vec{r} - \vec{r}') \psi^\pm(\vec{r}') d\vec{r}' d\vec{r} \\ &= \int \phi_b^*(\vec{r}) V(r) \psi^\pm(\vec{r}) d\vec{r} . \end{aligned} \quad 73$$

We know that $\phi_b = e^{+i\vec{k} \cdot \vec{r}}$; therefore 73 can be written as

$$T_{ba} = \frac{\hbar^2}{2m} \int e^{-i\vec{k} \cdot \vec{r}} U(r) \psi^\pm(\vec{r}) d\vec{r} . \quad 74$$

From the definition of $f(\theta)$ (eq. 71), we get

$$T_{ba} = - \frac{\hbar^2}{2m} 4\pi f(\theta) . \quad 75$$

In the forward direction, $\theta=0$, then

$$T_{aa} = - 2\pi \frac{\hbar^2}{m} f(0) . \quad 76$$

With $v_{\text{rel}} = \frac{k\hbar}{m}$, the optical theorem eq. 61 can be written as

$$\text{Im } f(0) = \frac{k}{4\pi} \sigma_{\text{T}} \quad 77$$

which is the familiar expression from quantum mechanics. The volume V does not appear in equation 77 because, for plane wave normalised to unity in unit volume, the incident flux is just v_{rel} and not $\frac{v_{\text{rel}}}{V}$.

CHAPTER II

NUCLEAR REACTIONS

An important branch of nuclear scattering is nuclear reactions in which a particle, under the influence of nuclear forces, is scattered elastically or inelastically. There has been an extensive study of this subject, both theoretical and experimental. The explanation given is either in terms of the formation of compound nucleus and resonances or of the direct reactions. In the latter case the examples are stripping and the pickup processes, where the incoming particle does not enter the nucleus and form compound nucleus but interacts with the loosely bound nucleons on the surface only. The nucleus is assumed to have a core, the incoming and outgoing particles have no interaction with nucleons inside this core. The nature of the interaction employed, of course, is short ranged.

Nuclear reactions involving compound nuclei are best understood in terms of Bohr's theory. The general treatment has been given by Wigner and Eisenbud^{12,B1,B13} in terms of the R matrix; no particular model is assumed for this theory. The elements of the R matrix are functions of energy, width and nuclear radius corresponding to a particular channel and these quantities

are taken to be adjustable parameters. Both the direct reactions and the theory of the R matrix have been omitted here; only the discussion based on the formation of the compound nucleus has been included. Whenever the term particle is used, it is assumed that it can be a simple particle or can have an internal structure.

Consider the particle a incident on the target nucleus X . Then the nuclear reaction may be written as

$$a + X = C$$

$$C = b + Y .$$

According to Bohr's postulates, a enters X , shares its energy with all other nucleons (the interaction being short ranged) and results in the excited nucleus C , the compound nucleus. Then C decays into the products b and Y (or more than two), the decay being absolutely independent of the mode of the formation of C . In the case of elastic scattering b is the same as a , and Y the same as X . For inelastic scattering b and Y can either be the same particles as a and X but in different quantum states, or b and Y may be entirely different from a and X .

Each pair or set of particles in a definite quantum state is said to represent a definite channel. Particles a and X form the entrance channel while b and Y form the exit channel. There can be more than one exit channel

for a reaction. However, which particular channels are open depends on the energy, angular momentum, parity etc.. Any particular interaction can be studied as a function of the energy of the incoming particle and the energies and directions of the outgoing particles.

Since most of the work on scattering can be found in nearly all quantum mechanics books, the unnecessarily detailed derivations will be avoided and only the essential expressions included. The calculations will be in the centre of mass system; for convenience, the tensor forces will be excluded.

a. Nuclear Cross Sections

The most important quantity determined in nuclear reactions is the nuclear cross section, elastic and inelastic. An important feature observed is the appearance of resonances i.e. sharp maxima in cross sections at certain energies. The knowledge of the cross sections helps in studying the reaction mechanism and nuclear structure. To start with, no special interior nuclear properties are assumed; the most important quantity employed to explain these cross sections is the logarithmic derivative of the wavefunction at the nuclear surface. Other nuclear properties viz. parities, angular momenta, energies, life times, etc. can then be determined.

Since we are using the centre of mass system, the co-ordinates used will be the relative co-ordinates and the reduced mass M of the two particles in the particular channel. The nuclear and particle spins will be neglected in sections IIa,b,d. For mathematical convenience, a plane wave is taken as the incident wave in the positive z -direction. Since it is independent of azimuthal angle ϕ , it can be expanded in terms of Legendre functions as

$$e^{ikz} = \sum_{\ell=0}^{\infty} i^{\ell} (2\ell+1) j_{\ell}(kr) P_{\ell}(\cos\theta) .$$

For large kr values i.e. $kr \gg 1$, substitute the asymptotic form of the Bessel function $j_{\ell}(kr)$, then

$$e^{ikz} = \sum_{\ell=0}^{\infty} \frac{(2\ell+1)}{2kr} i^{\ell+1} \left[e^{-i(kr - \frac{\ell\pi}{2})} - e^{+i(kr - \frac{\ell\pi}{2})} \right] P_{\ell}(\cos\theta). \quad 1$$

This is the undistorted wavefunction in the absence of any field. But when a potential is present, the outgoing part of the wave is changed. The total wavefunction in the entrance channel, α , then takes the form

$$\psi(\vec{r}) = \frac{\sqrt{\pi}}{kr} \sum_{\ell=0}^{\infty} \sqrt{2\ell+1} i^{\ell+1} \left[e^{-i(kr - \frac{\ell\pi}{2})} - \beta_{\ell} e^{+i(kr - \frac{\ell\pi}{2})} \right] Y_{\ell,0} \quad 2$$

where β_{ℓ} is the amplitude of the outgoing wave and depends on ℓ, k , and, of course, indirectly on the potential $V(r)$

If $V(r) = 0$, $\beta_\ell = 1$ and hence no scattering takes place. Because of the unitarity conditions, β_ℓ is in general a complex number. The condition that the outgoing flux does not exceed the incoming flux is

$$|\beta_\ell|^2 \leq 1 \quad . \quad 3$$

When $|\beta_\ell| = 1$, there is no reaction and when $\beta_\ell = 0$ there is maximum contribution to the reaction cross section as will be clear from the formulae derived below.

The scattered wave in channel α , which is the difference between the total wavefunction and the plane wave is given by

$$\psi_{sc}(\vec{r}) = \frac{\sqrt{\pi}}{kr} \sum_{\ell=0}^{\infty} \sqrt{2\ell+1} i^{\ell+1} (1-\beta_\ell) e^{i(kr - \frac{\ell\pi}{2})} Y_{\ell,0} \quad . \quad 4$$

Since $i^\ell = e^{i\ell\frac{\pi}{2}}$, equation 4 simplifies to

$$\psi_{sc}(\vec{r}) = \frac{1}{2kr} \sum_{\ell=0}^{\infty} (2\ell+1) i (1-\beta_\ell) e^{ikr} P_\ell(\cos\theta). \quad 5$$

In Chapter I, the asymptotic form of the scattered wave was derived (eq. 72). Therefore, we get the expression for scattering amplitude in terms of partial waves by comparing equations 5 and 72 (Chap. I)

$$f(\theta) = \frac{1}{2k} \sum_{\ell=0}^{\infty} i(2\ell+1)(1-\beta_\ell) P_\ell(\cos\theta) \quad . \quad 6$$

Summation over all ℓ 's corresponds classically to adding up all the impact parameters.

The number of particles N scattered or absorbed per second by a number N_i of the incident particles per unit area per second gives the scattering or the reaction cross section respectively. N is determined by

$$N = \frac{\hbar}{2im} \int \left(\frac{\partial \Psi}{\partial r} \Psi^* - \frac{\partial \Psi^*}{\partial r} \Psi \right) r_0^2 \sin\theta d\theta d\phi \quad 7$$

where r_0 is the radius of the large sphere through which the flux is being calculated. To calculate the scattering cross section, Ψ_{sc} from eq. 5 is used for the wavefunction in eq. 7 and for calculating the absorption cross section the total Ψ from eq. 2 is used.

The final results for the cross sections are^{B1}

$$\sigma_{sc,\ell} = \pi \chi^2 (2\ell+1) |1-\beta_\ell|^2 \quad 8$$

$$\sigma_{r,\ell} = \pi \chi^2 (2\ell+1) (1-|\beta_\ell|^2) \quad 9$$

where $\sigma_{sc,\ell}$ is the elastic scattering cross section and $\sigma_{r,\ell}$ is the reaction cross section for the ℓ^{th} partial wave. It is obvious from equation 9 that for reaction to take place $|\beta_\ell|^2 < 1$. Now $|\beta_\ell|^2$ enters $\sigma_{r,\ell}$ and β_ℓ , as a complex number, occurs in $\sigma_{sc,\ell}$; this corresponds to the fact that for inelastic scattering the outgoing and incoming waves are incoherent and hence there is no

interference while for elastic scattering the outgoing and incoming waves are coherent and they interfere.

[Interference treated in section IIId].

For calculating the angular distribution of the scattered particles the differential cross sections due to different partial waves cannot be added because different ℓ terms in one particular direction interfere. But when integrated over all the angles these interference terms disappear.

The β_ℓ depend on the nuclear structure and are determined from the properties of the wavefunction at the nuclear surface. The use of the latter property is possible due to the fact that Schrödinger equation is second order equation and the behaviour of the wavefunction and its derivative at the nuclear surface suffice to give complete information of β_ℓ . If it were a higher order equation then we would need additional conditions for a unique solution.

Let R be the sum of the radii of particle a and nucleus X , and $V(r)$ be the Coulomb potential energy between a and X at a separation $r > R$. With e as the electronic charge we have

$$V(r) = \frac{Z_a Z_x e^2}{r} .$$

If Ψ describes the relative motion of a and X , then it satisfies the equation

$$\nabla^2 \Psi(\vec{r}) + [k^2 - \frac{2M}{\hbar^2} V(r)] \Psi(\vec{r}) = 0 \quad r > R \quad . \quad 10$$

The radial wavefunction u_ℓ satisfies the equation

$$\frac{d^2 u_\ell(r)}{dr^2} + [k^2 - \frac{\ell(\ell+1)}{r^2} - \frac{2MV(r)}{\hbar^2}] u_\ell(r) = 0 \quad r > R \quad 11$$

with a regular solution $F_\ell(r)$ and irregular solution $G_\ell(r)$.

The asymptotic behaviour of these solutions is given by^{B1,B6,B12}

$$F_\ell(r) \rightarrow \sin(kr - \frac{\ell\pi}{2} + \sigma_\ell - \gamma \ln 2kr) \quad kr \gg \ell \quad 12$$

$$G_\ell(r) \rightarrow \cos(kr - \frac{\ell\pi}{2} + \sigma_\ell - \gamma \ln 2kr) \quad kr \gg \ell \quad 13$$

where σ_ℓ gives the Coulomb phase shift and

$$\gamma = \frac{Z_a Z_x e^2}{\hbar v} \quad .$$

Forming linear combinations of $F_\ell(r)$ and $G_\ell(r)$, we get

$$u_\ell^+(r) \equiv e^{-i\sigma_\ell} [G_\ell(r) + iF_\ell(r)] \equiv [u_\ell^-(r)]^* \quad 14$$

such that $u_\ell^+(r)$ represents an outgoing wave and $u_\ell^-(r)$, an incoming wave.[†]

[†] For neutrons, since $V(r) = 0$, $\sigma_\ell = 0$ and $\gamma = 0$, equations 12 and 13 are

$$F_\ell(r) \rightarrow \sin(kr - \frac{\ell\pi}{2})$$

$$G_\ell(r) \rightarrow \cos(kr - \frac{\ell\pi}{2})$$

and the solutions of eq. 11 are spherical Bessel functions ($F_\ell(r)$) and Neumann functions ($G_\ell(r)$).

Since the two solutions are linearly independent, the general solution of eq. 11 can be written as

$$u_{\ell}(r) = au_{\ell}^{(-)}(r) + bu_{\ell}^{(+)}(r) \quad . \quad 15$$

By comparing eq. 15 with eq. 2, the coefficients a and b are given by

$$a = i^{\ell+1} (2\ell+1) \frac{\sqrt{\pi}}{k} \quad , \quad b = -\beta_{\ell} a \quad . \quad 16$$

We introduce the well known quantities, f_{ℓ} , the logarithmic derivative, the real numbers Δ_{ℓ} and s_{ℓ} and the penetration factor v_{ℓ} as follows:

$$f_{\ell} \equiv R \left[\frac{du_{\ell}/dr}{u_{\ell}} \right]_{r=R} \quad 17$$

$$\Delta_{\ell} + is_{\ell} \equiv R \left[\frac{du_{\ell}^{(+)}/dr}{u_{\ell}^{(+)}} \right]_{r=R} \quad 18$$

$$v_{\ell} \equiv \frac{1}{G_{\ell}^2(R) + F_{\ell}^2(R)} \quad . \quad 19$$

The phase factor of $u_{\ell}^{(-)}(r)$ is defined by

$$e^{2i\xi_{\ell}} = \frac{u_{\ell}^{-}(R)}{u_{\ell}^{+}(R)} = \frac{G_{\ell}(R) - iF_{\ell}(R)}{G_{\ell}(R) + iF_{\ell}(R)} e^{2i\sigma_{\ell}} \quad 20$$

and therefore ξ_{ℓ} is real. In equations 17, 18, 19 and 20 it is understood that r approaches R from outside.

In terms of the quantities defined above, we get β_ℓ from equations 15 and 16 as

$$\beta_\ell = \frac{f_\ell - \Delta_\ell + i s_\ell}{f_\ell - \Delta_\ell - i s_\ell} e^{2i\xi_\ell} \quad . \quad 21$$

Equation 21 shows that the scattering cross section can be calculated without knowing the potential inside the nucleus; the only parameters required are the range R and the logarithmic derivative f_ℓ .

From equation 21, the requirement for a reaction to take place according to eq. 3 is that f_ℓ should be imaginary. If f_ℓ is real, $|\beta_\ell|^2 = 1$ and therefore the reaction cross section is zero.

Once the expression for β_ℓ is known, the cross section can be calculated from the quantities defined at the surface of the nucleus.

Substituting eq. 21 in eq. 8, the scattering cross section can be written as

$$\sigma_{sc,\ell} = (2\ell+1)\pi\chi^2 |A_{res}^\ell + A_{pot}^\ell|^2 \quad 22$$

where

$$A_{res}^\ell = \frac{-2is_\ell}{(\text{Re } f_\ell - \Delta_\ell) + i(\text{Im } f_\ell - s_\ell)} \quad 23$$

$$A_{pot}^\ell = e^{-2i\xi_\ell} - 1 \quad . \quad 24$$

A_{res}^{ℓ} is called the internal or resonance scattering amplitude. It gives the scattering due to internal effects of the nucleus. A_{pot}^{ℓ} does not contain any internal nuclear effects; it only gives scattering from a hard sphere. In the case of scattering from an impenetrable sphere, the wavefunction vanishes at $r = R$ and therefore $f_{\ell} = \infty$, which gives $A_{\text{res}}^{\ell} = 0$. Equation 22 shows that for elastic scattering there are three effects viz. resonance scattering, potential scattering and interference terms. The interference terms give rise to a minimum in the total cross section on the lower energy side of the resonance (section b).

Substitute eq. 21 in equation 9, then the reaction cross section is given by

$$\sigma_{r,\ell} = (2\ell+1)\pi\lambda^2 \frac{-4s_{\ell} \text{Im } f_{\ell}}{(\text{Re } f_{\ell} - \Delta_{\ell})^2 + (\text{Im } f_{\ell} - s_{\ell})^2} .$$

25

Because the cross section is a positive quantity, $\text{Im } f_{\ell} < 0$. From definitions 18 and 19 it can be shown that

$$s_{\ell} = kRv_{\ell} .$$

26

Since s_{ℓ} enters $\sigma_{r,\ell}$ in the numerator, it is clear that the greater the penetration factor v_{ℓ} , the greater the reaction cross section.

All these results will be generalised for spins and parities in section c.

b. Resonance Theory

At very high energies, the incident particle has a very small probability to escape through the entrance channel. We can say that the particle has been absorbed as far as the channel α is concerned. However, if the channel energy is low, the case is quite different. It is at these low energies that instead of observing a continuous spectrum, sharp peaks are observed in cross sections, which characterise resonance scattering.

To see qualitatively how resonances occur we consider a neutron inside the nucleus. The approximate shape of the potential assumed is that of a potential well with depth V_0 . If E is the kinetic energy of the neutron outside the nucleus, then the wave numbers outside and inside the nucleus are given respectively by

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad , \quad K = \sqrt{\frac{2m}{\hbar^2} (E + V_0)} \quad .$$

V_0 is usually 30-40 Mev and E usually less than 1 Mev so that $k \ll K$. The wavefunctions outside and inside can be approximately written as

$$u_{\text{out}} = B \cos kr$$

$$u_{\text{in}} = C \cos (Kr + \delta) \quad .$$

The logarithmic derivative is then

$$f_{\ell} = -KR \tan(KR + \delta) .$$

From the continuity of the wavefunctions and their derivatives at $r = R$ we get

$$\frac{C}{B} = \left[\frac{(KR)^2 + f_{\ell}^2}{(kR)^2 + f_{\ell}^2} \right]^{\frac{1}{2}} \frac{k}{K} . \quad 27$$

For $f_{\ell} \sim KR$, $\frac{C}{B} \propto \frac{k}{K}$. In other words, at low energies, the amplitude of the inside wavefunction is much smaller than the amplitude of the wavefunction outside the nucleus. Therefore, there is a small probability of the particle entering the nucleus. However, from equation 27 we see that maximum value of $\frac{C}{B}$ is 1 when $f_{\ell} = 0$. Therefore at certain particular energies ϵ_n , called the resonance energies, the phase shifts are just right to make the logarithmic derivative of the radial wavefunction zero at $r = R$. It is around these energies that the particle penetrates strongly into the nucleus and resonances in the formation of the compound nucleus are observed. At these low energies the cross section for the formation of the compound nucleus is no longer a monotonic function of energy. The compound nucleus formed has discrete states which, of course, are not stationary, but have a finite life time τ_n , characteristic of each state n .

The emission probability per unit time of the particle or photon from a particular resonance state n is

the reciprocal of the life time of that state. In energy units it can be written as

$$\Gamma^n = \frac{\hbar}{\tau_n}$$

and is called the width of the resonance state n . Any particular resonance level can decay by more than one different mode and each mode has its own characteristic life time or width. It is equivalent to saying that there is more than one exit channel open for the decay.

Therefore the total level width can be written as a sum of these different widths as follows:

$$\Gamma^n = \Gamma_{\text{rad}}^n + \sum_{\beta} \Gamma_{\beta}^n \quad 28$$

where β are the channels through which the level n can decay and Γ_{rad}^n gives the probability of decay of the level through photon emission.

To determine the cross sections at resonances, consider the approximate wavefunction inside the nucleus. It consists of an incoming wave and an outgoing wave; we can write it as

$$u(r) \sim e^{-iKr} + be^{+iKr} \quad r < R \quad . \quad 29$$

First consider elastic scattering in which case the coefficient b in eq. 29 just adds in a phase factor and we can write the wavefunction as

$$u(r) \sim C \cos (Kr + \delta) \quad r < R \quad 30$$

where δ is the phase shift and is a real number. At the resonance energy, the logarithmic derivative must vanish for $r = R$. Defining the formal resonance energy by ϵ_n , we have

$$f_\ell(\epsilon_n) = 0. \quad 31$$

A_{res} is of importance only when $f_0(\epsilon) < 1$; for $f_0(\epsilon) > 1$ it has been seen that $|A_{\text{res}}| < A_{\text{pot}}$. Therefore, for the general case we define an energy interval $\Delta\epsilon$, with $z(\epsilon) = (K(r) + \delta)$, by the condition

$$\tan z(\epsilon) < (KR)^{-1} \quad \text{for} \quad |\epsilon - \epsilon_n| < \Delta\epsilon.$$

Now $KR \gg 1$; therefore $\tan z(\epsilon)$ is small in the interval $\Delta\epsilon$. In this small energy interval we can assume a linear approximation and expand $f_\ell(\epsilon)$ around ϵ_n in a power series keeping only the first term. Then

$$f_\ell(\epsilon) = (\epsilon - \epsilon_n) \left(\frac{\partial f}{\partial \epsilon} \right)_n + \dots \quad 32$$

Introduce the following quantities: the channel width defined by^{*}

$$\Gamma_\alpha^n \equiv \frac{-2s_\ell(\epsilon)}{(\partial f_\ell / \partial \epsilon)_n} \quad 33$$

* Since we are dealing with a particular value of angular momentum, the index ℓ will be suppressed.

and the actual resonance energy

$$\epsilon_n' \equiv \epsilon_n + \frac{\Delta_\ell(\epsilon)}{\left(\frac{\partial \Gamma_\ell}{\partial \epsilon}\right)_n} . \quad 34$$

This factor Δ_ℓ appears due to the presence of Coulomb and centrifugal forces; it disappears for $\ell=0$ neutrons.

Γ_α^n and ϵ_n' are both functions of energy. With the help of equations 33 and 34, eq. 23 can be written as

$$A_{\text{res}}^\ell = \frac{i \Gamma_\alpha^n}{(\epsilon - \epsilon_n') + i \frac{1}{2} \Gamma_\alpha^n} \quad 35$$

which is the Breit Wigner one level formula. Comparing eqs. 24 and 35 we see that A_{res} and A_{pot} have opposite signs for $\epsilon < \epsilon_n$ and like signs for $\epsilon > \epsilon_n$. Consequently, a minimum in the total cross section is observed on the low energy side of the resonance due to interference of these two amplitudes.

All these calculations are based on a few assumptions. It is assumed that the function $z(\epsilon) = (KR + \delta)$ is a monotonic function of energy; $KR \gg 1$ so that $(\tan z(\epsilon))$ is extremely small in the energy interval $\Delta\epsilon$ and also that $\Delta\epsilon$ is much smaller than the level distance D . However, $\Delta\epsilon > \Gamma_\alpha^n$ for $kR \ll 1$.

In the case of a neutron with $\ell=0$, eq. 35 reduces to

$$A_{\text{res}} \approx \frac{i \Gamma_o^n}{(\epsilon - \epsilon_n) + i \frac{1}{2} \Gamma_o^n} \quad . \quad 36$$

In this case ϵ_n is constant while for charged particles ϵ_n' is a function of energy and hence the maximum for each level shifts with energy in the latter case.

Now consider the case when resonance reaction can also take place i.e. channels other than entrance channel are also open. Then the coefficient b in eq. 29 is a complex number; and the wavefunction inside the nucleus has the form

$$u_\ell(r) \sim C \cos(Kr + \delta + i\mu) \quad 37$$

where δ and μ are both real numbers and functions of the energy of the incoming particle. Since the outgoing wave can have an amplitude equal to or less than the amplitude of the incoming wave, $\mu \geq 0$. With eq. 37, the logarithmic derivative becomes

$$f_\ell = R \left[\frac{du_\ell/dr}{u} \right]_{r=R} = -KR \tan[z(\epsilon) + i\mu]. \quad 38$$

Now f_ℓ is complex and hence the reaction cross section is non-zero. Again, expanding $f_\ell(\epsilon)$ in the neighbourhood of ϵ_n we get

$$\begin{aligned} f_\ell(\epsilon) &\approx (\epsilon - \epsilon_n) \left(\frac{\partial f_\ell}{\partial \epsilon} \right)_n + \mu \left(\frac{\partial f_\ell}{\partial \mu} \right)_n \\ &\approx (\epsilon - \epsilon_n) \left(\frac{\partial f_\ell}{\partial \epsilon} \right)_n - i\mu KR. \end{aligned} \quad 39$$

Now define the particle width

$$\Gamma_{\alpha}^n \equiv - \frac{2 s_{\ell}(\epsilon)}{(\partial f_{\ell} / \partial \epsilon)_n} \quad 40$$

and reaction width

$$\Gamma_r^n \equiv - \frac{2\mu KR}{(\partial f_{\ell} / \partial \epsilon)_n} \quad 41$$

From equation 23 we get, after putting in these values, the resonance amplitude as

$$A_{res}^{\ell} = \frac{i \Gamma_{\alpha}^n}{(\epsilon - \epsilon_n') + i \frac{1}{2} \Gamma^n} \quad 42$$

where

$$\Gamma^n = \Gamma_r^n + \Gamma_{\alpha}^n$$

is the total width of the resonance level n . The elastic scattering cross section is still given by eq. 22 and the reaction cross section is given by the expression

$$\sigma_{r,\ell} = (2\ell+1) \pi \lambda^2 \frac{\Gamma_{\alpha}^n \Gamma_r^n}{(\epsilon - \epsilon_n') + (\frac{1}{2} \Gamma^n)^2} \quad 43$$

The difference between equations 36 and 42 is that in pure elastic scattering there is only Γ_{α}^n in the denominator for A_{res}^{ℓ} while eq. 42 has the total width Γ^n ; therefore the maximum forelastic scattering decreases in value when reactions are present. The denominator of σ_r does not depend on the entrance channel, but only on the properties of the nucleus.

Maxima, for both scattering and reaction cross sections occur at the same energy $\epsilon = \epsilon_n$.

This treatment of single level formulae is true when level distances are large. But when these distances are small, Kapur and Peierls have given the many level formula.^{B13,B6}

c. Spin, Orbital Angular Momentum and Parity

All the formulae derived in Sections IIa,b are for spinless particles. The only quantum number conserved in such cases was the orbital angular momentum ℓ . Now we introduce new quantum numbers: the total angular momentum J with z-component M , the particle spin s with z-component m_s , the nuclear spin I , and the channel spin S with z-component m_S . In the presence of nuclear spin I , particle spin s and orbital angular momentum ℓ , conservation of total angular momentum J has to be taken into account. Nuclear spin I and particle spin s form, by vector addition, the channel spin S . Then J can have the values $|\ell-S|, \dots, \ell+S$. For an unpolarised beam, for each value of S , there are $2S+1$ different channels (only unpolarised beams shall be treated below). For all values of S , the total number of states is $(2s+1)(2I+1)$. The statistical weight of a particular channel spin S is defined by

$$g(S) = \frac{2S+1}{(2s+1)(2I+1)} . \quad 44$$

For an unpolarised beam the contribution of all these $(2s+1)(2I+1)$ states adds incoherently. In each of these channels, ℓ combines with S to form J . In fact, each partial wave can be thought of as being a superposition of subwaves with different J values, $|\ell-S| \leq J \leq \ell+S$. Each ingoing wave is a pure ℓ wave, but the outgoing wave has different ℓ' values consistent with the same J , M and S values. (If the channel changes, then S changes too). The coefficient of the outgoing wave $-\beta_{\ell\ell'}(S,J)$ is the same for all $2S+1$ channels; different m_S values just imply different spatial orientations, the ratio of outgoing to ingoing amplitudes is the same.

The contribution of various ℓ waves with the same S, J, m_S is coherent and therefore they must be treated together. Hence, different wavefunctions $u(\ell, S, J, M; \vec{r})$ with the same J and S values are combined into one wavefunction $\omega(S, J, M; \vec{r})$ which is written as follows:

$$\omega(S, J, M; \vec{r}) = \sum_{\ell=|J-S|}^{J+S} u(\ell, S, J, M; \vec{r}) . \quad 45$$

On the other hand the contributions of various S waves are incoherent and therefore can be averaged over at the end. When there is a change in ℓ only and no change in S , we treat it as elastic scattering; however, whenever there is a change in S value, it is inelastic scattering.

The scattering cross section in eq. 8 is modified to^{B1}

$$\sigma_{sc}(S, J, M) = \pi \chi^2 \sum_{\ell' = |J-S|}^{J+S} \left| \sum_{\ell = |J-S|}^{J+S} i^{\ell+1} \sqrt{2\ell+1} C_{\ell S}(J, M; 0, m_S) \right. \\ \left. \times [\delta_{\ell\ell'} - \beta_{\ell\ell'}(S, J)] \right|^2 \quad 46$$

where $C_{\ell S}(J, M; 0, m_S)$ are the Clebsch-Gordan coefficients with $m_\ell = 0$. Averaging over the $2S+1$ m_S values, eq. 46 simplifies to

$$\sigma_{sc}(S, J) = \frac{2J+1}{2S+1} \pi \chi^2 \sum_{\ell, \ell' = |J-S|}^{J+S} \left| \delta_{\ell\ell'} - \beta_{\ell\ell'}(S, J) \right|^2 \quad 47$$

on account of the relation

$$\sum_{M=-J}^J \sum_{m_S=-S}^S C_{\ell S}^*(J, M; 0, m_S) C_{\ell' S}(J, M; 0, m_S) = \frac{2J+1}{2\ell+1} \delta_{\ell\ell'} .$$

Instead of eq. 9, the reaction cross section for channel spin S and total angular momentum J now has the following expression^{B1}

$$\sigma_r(S, J) = \frac{2J+1}{2S+1} \pi \chi^2 \sum_{\ell, \ell' = |J-S|}^{J+S} (\delta_{\ell\ell'} - |\beta_{\ell\ell'}|^2) . \quad 48$$

When $\ell \neq 0$, then all those channel spins, which, together with the ℓ values from the same J value, contribute to the same resonance state. However, when $\ell = 0$, different

channels have different J values and hence form different resonance states. Although there is no contribution to the resonance scattering cross section from non-resonance channel spins, the potential scattering amplitude does get a contribution.

The next important quantum number to be included is the parity π which is conserved in general (except for weak interactions) in nuclear reactions. The parity $\pi(a)$ of particle a does not depend on its spin orientation and $\pi(X)$, parity of X , does not depend on the direction of its nuclear spin I . The parity of the wavefunction describing the relative motion of a and X depends on the ℓ value; even for even ℓ and odd for odd ℓ . Therefore, if parity is to be conserved, ℓ must change by an even number during scattering. We know that at low energies, for elastic scattering, we normally encounter low ℓ values. Therefore, if $\Delta\ell$ is to be even, only $\Delta\ell=0$ is likely to occur. Consequently, elastic scattering with $\ell' \neq \ell$ can be neglected. But, at higher energies and for inelastic scattering there could be a change in ℓ value.

If X is in the quantum state α' with parity $\pi_{\alpha'}$, and a in the quantum state α'' with parity $\pi_{\alpha''}$, then the channel parity is defined as

$$\pi_{\alpha} = \pi_{\alpha'} \pi_{\alpha''}$$

and the parity of the compound nucleus as

$$\pi_c = (-1)^{\ell} \pi_{\alpha}.$$

Introduce the quantity $\omega_{\ell}(\pi)$ by

$$\omega_{\ell}(\pi) = \frac{1}{2} [1 + (-1)^{\ell} \pi] \quad , \quad 49$$

which is clearly unity for $(-1)^{\ell} = \pi$ and zero for $(-1)^{\ell} = -\pi$.

For channel spin S , total angular momentum J and parity π_c , we replace eqs. 47 and 48 by^{B1}

$$\sigma_{sc}(S, J, \pi_c) = \frac{2J+1}{2S+1} \pi \lambda^2 \sum_{\ell, \ell' = |J-S|}^{J+S} \omega_{\ell}(\pi_{\alpha} \pi_c) \omega_{\ell'}(\pi_{\alpha} \pi_c) |\delta_{\ell \ell'} - \beta_{\ell \ell'}(S, J, \pi_c)|^2 \quad 50$$

$$\sigma_r(S, J, \pi_c) = \frac{2J+1}{2S+1} \pi \lambda^2 \sum_{\ell, \ell' = |J-S|}^{J+S} \omega_{\ell}(\pi_{\alpha} \pi_c) \omega_{\ell'}(\pi_{\alpha} \pi_c) \times (\delta_{\ell \ell'} - |\beta_{\ell \ell'}|^2) \quad 51$$

For unpolarised beams, formulae 50 and 51 become

$$\sigma_{sc,r} = \sum_{\pi_c = \pm 1} \sum_{J=0}^{\infty} \sum_{S=|I-S|}^{I+S} g(S) \sigma_{sc,r}(S, J, \pi_c) \quad 52$$

with the condition of conservation of flux

$$\sum_{\ell' = |S-J|}^{S+J} |\beta_{\ell \ell'}(S, J, \pi_c)|^2 \leq 1 \quad . \quad 53$$

Now consider the resonance region. Since ℓ does not have a fixed value, $|J-S| \leq \ell \leq J+S$, each partial width $\Gamma_{\alpha\ell}^n$ has to be specified with the particular orbital angular momentum. The level separation now is the distance between levels of the compound nucleus with the same J and π_c values. The reaction cross section $\sigma(\alpha_S, \beta_{S'})$ is given by

$$\sigma(\alpha_S, \beta_{S'}) = \pi\chi^2 \frac{2J+1}{(2s+1)(2I+1)} \times \sum_{\ell=|J-S|}^{J+S} \sum_{\ell'=|J-S'|}^{J+S'} \omega_{\ell}(\pi_{\alpha}\pi_c) \omega_{\ell'}(\pi_{\beta}\pi_c) \frac{\Gamma_{\alpha\ell}^n \Gamma_{\beta\ell'}^n}{(\epsilon - \epsilon_n)^2 + (\frac{1}{2}\Gamma^n)^2}$$

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where Γ^n is the total width of the level. If $\pi_{\alpha} = \pi_{\beta}$, then ℓ' of the outgoing particles is even (odd) if ℓ of the incoming particles is even (odd). For $\pi_{\alpha} = -\pi_{\beta}$, the outgoing ℓ' is even (odd) if the incoming ℓ is odd (even). The parity of the entrance channel, π_{α} is the same as the parity of the ground state of X and the parity of the exit channel, π_{β} is the same as the ground state of the residual nucleus Y .

The elastic scattering cross section for neutrons near a resonance with angular momentum J , parity π_c , produced by parity π_{α} with particles of spin s and I is given by^{B1} -

$$\begin{aligned}
\sigma_{sc} &= \pi \lambda^2 \frac{2J+1}{(2S+1)(2I+1)} \\
&\times \left\{ \sum_{S=|I-S|}^{I+S} \sum_{\ell=|J-S|}^{J+S} \omega_{\ell}(\pi_{\alpha} \pi_c) \left| \frac{i \Gamma_{\alpha \ell}^n}{\epsilon - \epsilon_n + i \frac{1}{2} \Gamma^n} + A_{pot}^{\ell} \right|^2 \right. \\
&+ \sum_{S=|I-S|}^{I+S} \sum_{\ell \neq \ell'=|J-S|}^{J+S} \omega_{\ell}(\pi_{\alpha} \pi_c) \omega_{\ell'}(\pi_{\alpha} \pi_c) \frac{\Gamma_{\alpha \ell}^n \Gamma_{\alpha \ell'}^n}{(\epsilon - \epsilon_n)^2 + (\frac{1}{2} \Gamma^n)^2} \\
&+ \sum_{S \neq S'=|I-S|}^{I+S} \sum_{\ell=|J-S|}^{J+S} \sum_{\ell'=|J-S'|}^{J+S'} \omega_{\ell}(\pi_{\alpha} \pi_c) \omega_{\ell'}(\pi_{\alpha} \pi_c) \\
&\times \frac{\Gamma_{\alpha \ell}^n \Gamma_{\alpha \ell'}^n}{(\epsilon - \epsilon_n)^2 + (\frac{1}{2} \Gamma^n)^2} + \frac{(2S+1)(2I+1)}{2J+1} \sum_{\ell=0}^{\infty} (2\ell+1) |A_{pot}^{\ell}|^2 \\
&\left. - \sum_{S=|I-S|}^{I+S} \sum_{\ell=|J-S|}^{J+S} \omega_{\ell}(\pi_{\alpha} \pi_c) |A_{pot}^{\ell}|^2 \right\}. \tag{55}
\end{aligned}$$

This formula gives the total scattering cross section for an isolated resonance integrated over all angles and summed and averaged over all spin directions. The expression for charged particles also includes Rutherford scattering and is quite complicated. The first term in eq. 55 gives resonance scattering without change of ℓ and S . The second term gives resonance scattering with change of ℓ but without change of S . This term is of hardly any importance. The third term which allows change of S , vanishes for parity favoured reactions, but is of great importance

for parity unfavoured reactions. The fourth term gives the contribution due to potential scattering at off-resonance energies while the last term subtracts the contribution of potential scattering at resonance energies.

Thus we see that these formulae become more and more complicated with the inclusion of more quantum numbers. In practice, the simple cases usually treated give equally important information.

d. Interference

In section IIa, it has been shown that the incoming and the scattered waves are coherent for elastic scattering. But in actual calculations the interference contribution is never accounted for. The justification for this follows.

The asymptotic wavefunction in scattering (Chap. I, eq. 72) is given by

$$\psi = e^{+ikz} + \frac{e^{-ikr}}{r} f(\theta, \phi) \quad 56a$$

with

$$\psi^* = e^{-ikz} + \frac{e^{-ikr}}{r} f^*(\theta, \phi) . \quad 56b$$

The flux per unit area at the surface of a very large sphere is given by

$$\begin{aligned}
J_n &= \frac{\hbar}{2im} \left(\Psi^* \frac{\partial \Psi}{\partial r} - \Psi \frac{\partial \Psi^*}{\partial r} \right) \\
&= \frac{\hbar}{2im} \left[(e^{-ikz} + \frac{e^{-ikr}}{r} f^*(\theta, \phi)) \right. \\
&\quad \times (ik \cos \theta e^{ikz} + \frac{ik}{r} e^{ikr} f(\theta, \phi) - \frac{e^{ikr}}{r^2} f(\theta, \phi)) \\
&\quad - (e^{ikz} + \frac{e^{ikr}}{r} f(\theta, \phi)) \\
&\quad \times (-ik \cos \theta e^{ikz} - \frac{ik}{r} e^{-ikr} f^*(\theta, \phi) - \frac{e^{-ikr}}{r^2} f^*(\theta, \phi)) \left. \right] \\
J_n &\approx \frac{\hbar}{2im} \left[2ik \cos \theta + \frac{ik}{r} e^{-ikz+ikr} f\{1 + \cos \theta\} \right. \\
&\quad + \frac{ik}{r} e^{ikz-ikr} f^*\{1 + \cos \theta\} \\
&\quad - \frac{1}{r^2} \{e^{-ikz+ikr} f - e^{ikz-ikr} f^*\} + \frac{2ik}{r^2} |f|^2 \left. \right] \\
&= \frac{\hbar}{m} k \cos \theta + \frac{\hbar k}{m} \frac{|f|^2}{r^2} + \frac{k\hbar}{2mr} (1 + \cos \theta) \{f e^{ikr(1-\cos \theta)} + \text{c.c.}\} \\
&\quad - \frac{\hbar}{2imr^2} \{f e^{ikr(1-\cos \theta)} - \text{c.c.}\}
\end{aligned} \tag{57}$$

where c.c. is the complex conjugate of the previous term. The first term in eq. 57 is due to the incident plane wave, the second term, after integration, will give the scattered wave, while the last two terms are the interference terms in which we are interested.

Consider the contribution of the interference terms into a solid angle $\Delta\Omega$ at a distance r_0 (radius of the large sphere being considered). We get

$$\begin{aligned} & \frac{kh}{2mr_0} \frac{1}{\Delta\Omega} \int_{\theta}^{\theta+\Delta\theta} \int_{\phi}^{\phi+\Delta\phi} (1+\cos\theta) \{f(\theta, \phi) e^{ikr(1-\cos\theta)} + \text{c.c.}\} \\ & \times r_0^2 \sin\theta d\theta d\phi - \frac{\hbar}{2imr_0^2} \frac{1}{\Delta\Omega} \int_{\theta}^{\theta+\Delta\theta} \int_{\phi}^{\phi+\Delta\phi} \\ & \times \{ f e^{ikr(1-\cos\theta)} - \text{c.c.} \} r_0^2 \sin\theta d\theta d\phi . \end{aligned}$$

Neglecting the ϕ dependence because of cylindrical symmetry and putting $\cos\theta = \mu$, the above expression simplifies to

$$\begin{aligned} & \frac{kr_0 \hbar}{2m} \frac{1}{\Delta\mu} \int_{\mu}^{\mu+\Delta\mu} (1+\mu) \{ f e^{ikr_0(1-\mu)} + \text{c.c.} \} d\mu \\ & - \frac{\hbar}{2im} \frac{1}{\Delta\mu} \int_{\mu}^{\mu+\Delta\mu} \{ f e^{ikr_0(1-\mu)} - \text{c.c.} \} d\mu . \end{aligned}$$

We assume that f is a continuous, slowly varying function of the angle variables. In the asymptotic region we are justified in choosing kr_0 large enough so that $e^{ikr_0(1-\mu)}$ is a rapidly oscillating function. Then its average over the interval $\Delta\mu$ is zero. Thus we see that the contribution of the interference terms in the asymptotic region is zero unless $\theta = 0$. In the incident direction the

exponential is unity; consequently there is no oscillating part and the integrand is just a constant.

In the beginning of Chapter I it was pointed out that instead of plane waves, wave packets are actually used and, therefore, there is always a spread in the k value. We can integrate eq. 57 from k to $k+\Delta k$. Again because of large r_0 value, the exponential function is rapidly oscillating and its average over the interval Δk yields zero except when $\theta = 0$. Hence, by this method also, we find the contribution of the interference terms zero at all angles except when $\theta = 0$.

CHAPTER III

VARIATIONAL PRINCIPLE AND SCATTERING

In Chapters I and II expressions for scattering cross sections have been derived. However, it is more advantageous to determine phase shifts rather than cross sections, since mathematically, the latter are expressed in terms of the former. Except for the direct integration of the Schrödinger equation in a very few simple cases, an exact analytic expression for these quantities is not possible. Therefore some approximate expressions have been devised which have quite a high degree of accuracy. The Born approximation is one of these methods which is applicable for weak fields only. The other is the well known variational method with the help of which the stationary value of the quantity involved can be determined to quite a good accuracy.

Different variational techniques have been given by various workers. The first order terms are found to be the same in all cases; deviations lie in the second and higher order terms. The main objective behind all methods is to keep the higher order terms as small as possible. Variational expressions for phase shifts and scattering amplitudes will be discussed in this chapter; a few of the important applications will follow in Chapter IV.

The time independent Schrödinger equation for scattering of particles with energy $E = \frac{\hbar^2 k^2}{2m}$ by a potential $V(\vec{r}) = \frac{\hbar^2}{2m} U(\vec{r})$ is

$$\{\nabla^2 + k^2 - U(\vec{r})\}\Psi(\vec{r}) = 0 \quad . \quad 1$$

The required asymptotic form of the wavefunction should be (according to Chap. I)

$$\Psi(\vec{r}) \sim e^{i\vec{k} \cdot \vec{r}} + \frac{e^{ikr}}{r} f(\theta, \phi) \quad . \quad 2$$

For spherically symmetrical potentials, we can take the incident beam along the z-axis so that all the expressions are independent of azimuthal angle ϕ ; in that case we can expand $\Psi(\vec{r})$ in terms of Legendre polynomials:

$$\Psi(\vec{r}) = \sum_{\ell=0}^{\infty} A_{\ell} \frac{u_{\ell}(r)}{r} P_{\ell}(\cos\theta) \quad . \quad 3$$

The $u_{\ell}(r)$ satisfy the radial equation

$$\frac{d^2 u_{\ell}(r)}{dr^2} + \{k^2 - U(r) - \frac{\ell(\ell+1)}{r^2}\} u_{\ell}(r) = 0 \quad . \quad 4$$

The solution of this equation must obey the boundary conditions

$$u_{\ell}(0) = 0$$

$$u_{\ell}(r) \xrightarrow{r \rightarrow \infty} \frac{1}{k} \sin(kr - \frac{\ell\pi}{2} + \eta_{\ell}) \quad 5$$

where η_ℓ is the phase shift for the ℓ^{th} partial wave. Spin, parity and other internal nuclear quantum numbers are being neglected throughout Chapters III and IV.

Other different normalisations possible for $u_\ell(r)$ are

$$u_\ell(r) \sim \sin(kr - \frac{\ell\pi}{2}) + \tan\eta_\ell \cos(kr - \frac{\ell\pi}{2}), \quad 6$$

$$u_\ell(r) \sim \cot\eta_\ell \sin(kr - \frac{\ell\pi}{2}) + \cos(kr - \frac{\ell\pi}{2}) . \quad 7$$

The phase shifts η_ℓ , $\tan\eta_\ell$ or $\cot\eta_\ell$ are functions of $U(r)$, k and ℓ .

a. Hulthén's Variational Principle for Phase Shifts

This was one of the first variational principles formulated in the theory of scattering. Introducing the differential operator

$$L \equiv \frac{d^2}{dr^2} + k^2 - U(r) - \frac{\ell(\ell+1)}{r^2} . \quad 8$$

Equation 4 can be written as

$$Lu(r) = 0 . \quad 9$$

Define the functional

$$I(v) = \int_0^\infty vLv \, dr \quad 10$$

where v is an arbitrary quadratically integrable function of r . If v happens to be the exact solution of the radial

wave equation u , then

$$I(u) = 0 \quad 11$$

where $u(r)$ vanishes at the origin and has the asymptotic form given by eq. 5. Consider the function $u+\delta u$, differing infinitesimally from u , vanishing at $r = 0$ and

$$u+\delta u \underset{r \rightarrow \infty}{\sim} \frac{1}{k} \sin(kr - \frac{\ell\pi}{2} + \eta_\ell + \delta\eta_\ell) . \quad 12$$

Hence, it follows that δu for large r has the form

$$\delta u \underset{r \rightarrow \infty}{\sim} \frac{1}{k} \cos(kr - \frac{\ell\pi}{2} + \eta_\ell) \delta\eta_\ell . \quad 13$$

The variation in $I(u)$ is given by

$$\begin{aligned} \delta I(u) &= \int_0^\infty \delta u L u dr + \int_0^\infty u L \delta u dr + \int_0^\infty \delta u L \delta u dr \\ &\approx 2 \int_0^\infty \delta u L u - \frac{1}{k} \delta\eta_\ell . \end{aligned}$$

We have neglected terms of second order in infinitesimal quantities. Since $Lu = 0$, we get

$$\delta I(u) = - \frac{1}{k} \delta\eta_\ell , \quad 14$$

which is Hulthén's variational principle. According to Hulthén, choose the trial function such that $\delta I(u) = 0$ which leads to the stationary property of the phase shift.

Select a trial function $u_T(r)$ which is continuous and bounded for all r , satisfying the boundary conditions

$$u_T(0) = 0 \quad 15a$$

$$u_T(r) \underset{r \rightarrow \infty}{\sim} \frac{1}{k} \sin(kr - \frac{\ell\pi}{2} + \eta_T) \quad 15b$$

and which depends on n parameters c_i ($i=1,2,\dots,n$) and η_T . Then $u_T(r)$ is substituted for v in $I(v)$ and the $(n+1)$ parameters are determined from $(n+1)$ equations

$$I_T = 0 \quad \frac{\partial I_T}{\partial c_i} = 0 \quad i=1,2,\dots,n \quad 16$$

where $I_T = I(u_T)$. Using these values of $(n+1)$ parameters, approximate values of $u(r)$ and η_ℓ are determined. Usually four parameters have been seen to be sufficient for energies less than 10 Mev. The complication of the form of the trial wave function depends on how many types of fields and perturbing forces have to be included.

If we choose the normalisations given by equations 6 and 7, then instead of eq. 14 we get

$$\delta(kI - \tan\eta_\ell) = 0 \quad 17$$

$$\delta(kI + \cot\eta_\ell) = 0 \quad 18$$

As one can see in the above argument a unique value of u cannot be obtained since I is a quadratic function

of u . We will now discuss Kohn-Hulthén method, which has been introduced to overcome this difficulty.

Define the functional

$$F = \lambda + kI_{\ell} = \lambda + k \int_0^{\infty} vLv \, dr$$

where $\lambda = \eta_{\ell}$, $\tan\eta_{\ell}$ or $-\cot\eta_{\ell}$ depending on the normalisations used. The stationary value of F is then η_{ℓ} , $\tan\eta_{\ell}$ or $-\cot\eta_{\ell}$ respectively. To determine $(n+1)$ parameters, the Kohn-Hulthén conditions are given by the following $(n+1)$ equations

$$\frac{\partial F}{\partial \lambda} = 0 \quad \frac{\partial F}{\partial c_i} = \frac{\partial I_{\ell}}{\partial c_i} = 0 \quad (i=1,2,\dots,n). \quad 19$$

Here we do not get quadratic expressions in the functional of η_{ℓ} because the first condition is modified. However, it has been observed that if Hulthén's method and the Kohn-Hulthén method are applied together to give the same value of η_{ℓ} consistently, then the lower value of the two solutions of the quadratic equation must be chosen.

b. Kato's Variational Principle for Phase Shifts

Kato has taken a more general expression for the asymptotic form of the wavefunction by introducing a constant θ , which is left at our disposal. Let the asymptotic form of the solution of $Lu=0$ be

$$u(r) \underset{r \rightarrow \infty}{\sim} \cos(kr - \frac{\ell\pi}{2} + \theta) + \alpha \sin(kr - \frac{\ell\pi}{2} + \theta)$$

20

with $u(0) = 0$ and

$$\alpha = \cot(\eta - \theta) .$$

Introducing an infinitesimal change δu in u , we obtain

$$\delta u \underset{r \rightarrow \infty}{\sim} \delta \alpha \sin(kr - \frac{\ell\pi}{2} + \theta) \quad 21$$

and therefore

$$\begin{aligned} \delta I(u) &= \int_0^{\infty} \delta u L u dr + \int_0^{\infty} u L \delta u dr + \int_0^{\infty} \delta u L \delta u dr \\ &= k \delta \alpha + \int_0^{\infty} \delta u L \delta u dr . \end{aligned}$$

Neglecting the second term on the R.H.S., we get

$$\delta I(u) \approx k \delta \alpha , \quad 22a$$

which is Kato's variational principle. It gives Hulthén's form if we choose $\theta = \frac{\pi}{2}$ and $\alpha = -\tan \eta$. The functional

$$F(v) = k\zeta - \int_0^{\infty} v L v dr \quad 22b$$

with $v(0) = 0$

$$v(r) \underset{r \rightarrow \infty}{\sim} \cos(kr - \frac{\ell\pi}{2} + \theta) + \zeta \sin(kr - \frac{\ell\pi}{2} + \theta)$$

is stationary for $v = u$ and the stationary value of F is

$$F(u) = k\alpha .$$

Kato^{8a} has shown, by giving different values to θ and α , that all variational principles (sections a,b,c, d) are mathematically equivalent. In Chap. IV Kato's method has been used to demonstrate the monotonic property of phase shifts.

c. Tamm's Variational Principle

In the previous methods, the asymptotic form of the radial wavefunction was expressed in terms of phase shifts and energies. Tamm^{B5,3a} introduced another function $g(r)$ as follows:

$$u(r) = kr\{j_\ell(kr) - \alpha g(r)n_\ell(kr)\} \quad 23$$

for all r ; and $\alpha = \tan\eta$. To determine the boundary conditions on $g(r)$, assume that $U(r)$ is less singular than r^{-2} at the origin. Then, as $r \rightarrow 0$

$$u(r) \longrightarrow r^{\ell+1} .$$

Also since $n_\ell(kr) \longrightarrow r^{-\ell-1}$ for small r , we must have

$$g(r) \sim r^{2\ell+1}$$

for small r . From the asymptotic form of $u(r)$ and the properties of $j_\ell(kr)$ and $n_\ell(kr)$ for large r , we obtain

$$g(r) \sim 1 \quad \text{for large } r.$$

Thus the trial wavefunction now depends on two parameters, α_T and $g_T(r)$; it can be written as

$$u_T(r) = k\{j_\ell(kr) - \alpha_T g_T(r) n_\ell(kr)\} \quad 24$$

for all r and

$$g_T(r) \sim r^{2\ell+1} \quad \text{for small } r$$

$$g_T(r) \sim 1 \quad \text{for large } r.$$

Substitute u_T (eq. 23) for v in $I(v)$ and integrate by parts. After long calculations and using the recurrence relations for $j_\ell(kr)$ and $n_\ell(kr)$ we arrive at the relation

$$\begin{aligned} \alpha_T + \frac{1}{k} I_T = & -k \left[\alpha_T^2 \int_0^\infty r^2 \{n_\ell(kr)\}^2 \left(\frac{dg_T}{dr}\right)^2 dr \right. \\ & \left. + \int_0^\infty r^2 \{j_\ell(kr) - \alpha_T g_T(r) n_\ell(kr)\}^2 U(r) dr \right]. \end{aligned}$$

Differentiating the above equation with respect to α_T and using Kohn's first condition $\frac{\partial I_T}{\partial \alpha_T} = 0$, we get the expression for α_T .

$$\alpha_T = \frac{\int_0^\infty r^2 j_\ell(kr) n_\ell(kr) g_T(r) U(r) dr}{\int_0^\infty r^2 \{n_\ell(kr)\}^2 g_T^2(r) U(r) + \left(\frac{dg_T}{dr}\right)^2 dr}.$$

With this value of α_T we get

$$\alpha_T + \frac{1}{k} I_T = \tan \eta_B + \alpha_T k \int_0^{\infty} r^2 j_{\ell}(kr) n_{\ell}(kr) g_T(r) \times U(r) dr \quad 25$$

where

$$\tan \eta_B = -k \int_0^{\infty} r^2 \{j_{\ell}(kr)\}^2 U(r) dr$$

is the Born approximation to the phase shift. Equation 25 can be further simplified to

$$\alpha_T + \frac{1}{k} I_T = - \int_0^{\infty} r j_{\ell}(kr) u_T(r) U(r) dr . \quad 26$$

The R.H.S. of equation 26 is the integral expression for the phase shifts^{B13}, $u(r)$ replaced by $u_T(r)$. Thus when $u_T(r)$ is an exact solution, then $I_T = 0$ and equation 26 gives the exact value of $\tan \eta$.

Using the same trial wavefunctions, Tamm has shown that his method gives better values than that of Hulthén.

d. Schwinger's Variational Principle for Phase Shifts

Schwinger gave another method which gives the stationary value of phase shifts directly and the trial wavefunctions do not have to be normalised. This method will be discussed in detail as applied to time independent and time dependent theory of scattering.

The Green's function for the equation

$$\left\{ \frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2} \right\} G(r, r') = -\delta(r-r') \quad 27$$

is given by^{B5, B12, B13}

$$G(r, r') = -kr_{<}r_{>}j_{\ell}(kr_{<})n_{\ell}(kr_{>}) \quad 28$$

where $r_{<}$ and $r_{>}$ are the lesser or greater of r and r' . The asymptotic form of the radial wavefunction $u_{\ell}(r)$ is chosen as^{7a}

$$u_{\ell}(r) \underset{r \rightarrow \infty}{\sim} kr\{j_{\ell}(kr) - \tan\eta_{\ell} n_{\ell}(kr)\} . \quad 29$$

The general solution of eq. 4 is given by

$$\begin{aligned} u_{\ell}(r) &= krj_{\ell}(kr) - \int_0^{+\infty} G(r, r')U(r')u_{\ell}(r')dr' \\ &= krj_{\ell}(kr) + \int_0^{\infty} kr_{<}r_{>}j_{\ell}(kr_{<})n_{\ell}(kr_{>})U(r')u(r')dr'. \end{aligned} \quad 30$$

Comparing equations 29 and 30 we get

$$\tan\eta_{\ell} = - \int_0^{\infty} r'j_{\ell}(kr')U(r')u(r')dr' . \quad 31$$

Multiply eq. 30 by $U(r)u(r)$ and integrate, it gives

$$\begin{aligned} \int_0^{\infty} krj_{\ell}(kr)U(r)u_{\ell}(r)dr &= \int_0^{\infty} U(r)\{u_{\ell}(r)\}^2dr \\ &+ \int_0^{\infty} U(r)u_{\ell}(r)dr \int_0^{\infty} G(r, r')U(r')u_{\ell}(r')dr' . \end{aligned} \quad 32$$

Hence with the aid of equation 31 we get

$$k \cot \eta_{\ell} = - \frac{\int_0^{\infty} U(r) \{u_{\ell}(r)\}^2 dr + \int_0^{\infty} U(r) u_{\ell}(r) dr \int_0^{\infty} G(r, r') U(r') u_{\ell}(r') dr'}{\left\{ \int_0^{\infty} r j_{\ell}(kr) U(r) u_{\ell}(r) dr \right\}^2} \quad 33$$

which is Schwinger's variational expression for phase shifts.

The function which satisfies the Schrödinger equation is exactly the function which makes eq. 30 stationary. Conversely, the value of $k \cot \eta_{\ell}$ computed from that function $u(r)$ which makes 30 stationary will give the correct phase shifts. To verify this, replace $u(r)$ by $u(r) + \delta u(r)$ in eq. 33, expand in terms linear in $\delta u(r)$ and put

$$k \cot \eta_{\ell} = J(u) \quad . \quad 34$$

Then we get

$$\begin{aligned} (J + \Delta J) & \left[\int_0^{\infty} r j_{\ell}(kr) U(r) \{u_{\ell}(r) + \delta u_{\ell}(r)\} dr \right]^2 \\ &= - \int_0^{\infty} U(r) \{u_{\ell}(r) + \delta u_{\ell}(r)\}^2 dr \\ &\quad - \int_0^{\infty} U(r) \{u_{\ell}(r) + \delta u_{\ell}(r)\} dr \\ &\quad \times \int_0^{\infty} G(r, r') U(r') \{u_{\ell}(r') + \delta u_{\ell}(r')\} dr' \end{aligned}$$

or

$$\begin{aligned}
& (J + \Delta J) \left\{ \int_0^\infty r j_\ell(kr) U(r) u_\ell(r) dr \right\}^2 \\
& + 2 \int_0^\infty r j_\ell U(r) u_\ell(r) dr \int_0^\infty r j_\ell U(r) \delta u_\ell(r) dr \\
& = - \int_0^\infty U(r) \{u_\ell(r)\}^2 dr - 2 \int_0^\infty U(r) u_\ell(r) \delta u_\ell(r) dr \\
& - 2 \int_0^\infty U(r) \delta u_\ell(r) dr \int_0^\infty G(r, r') U(r') u_\ell(r') dr' \\
& - \int_0^\infty U(r) u_\ell(r) dr \int_0^\infty G(r, r') U(r') u_\ell(r') dr'
\end{aligned}$$

or

$$\begin{aligned}
& 2J \int_0^\infty r j_\ell U(r) u_\ell(r) dr \int_0^\infty r j_\ell U(r) \delta u_\ell(r) dr \\
& + \Delta J \left[\int_0^\infty r j_\ell(kr) U(r) u_\ell(r) dr \right]^2 \\
& = - 2 \int_0^\infty U(r) u_\ell(r) \delta u_\ell(r) dr \\
& - 2 \int_0^\infty U(r) \delta u_\ell(r) dr \int_0^\infty G(r, r') U(r') u_\ell(r') dr' .
\end{aligned}$$

Since $\delta u_\ell(r)$ is arbitrary, we put the coefficient of $\delta u_\ell(r)$ equal to zero. Then

$$\begin{aligned}
J \int_0^\infty r j_\ell U(r) u_\ell(r) dr \int_0^\infty r j_\ell U(r) \delta u_\ell(r) dr & = -U(r) u_\ell(r) - U(r) \int_0^\infty G(r, r') U(r') \\
& \times u_\ell(r') dr' .
\end{aligned}$$

With $J = k \cot \eta$

$$= \frac{k}{\tan \eta} = - \frac{k}{\int_0^\infty r j_\ell(kr) U(r) u_\ell(r) dr}$$

we get

$$-krj_{\ell}(kr) = -u(r) - \int_0^{\infty} G(r,r')U(r')u(r')dr'$$

or

$$u(r) = krj_{\ell}(kr) - \int_0^{\infty} G(r,r')U(r')u(r')dr'$$

which is the same as eq. 30.

It is obvious from eq. 33 that the normalisation of $u(r)$ is not required since the R.H.S. is uniform in the powers of $u(r)$. Furthermore, any error in $k \cot \eta$ occurs as the square of the error in $u(r)$. Since $u(r)$ appears in the expression in the combination $U(r)u(r)$, the error is important only within the nuclear range. The main difficulty in Schwinger's method is the calculation of double integral.

Schwinger^{6a} also gives a method for improving the trial wavefunction systematically. Starting with a trial wavefunction $u_0(r)$ in eq. 33 we get $k \cot \eta_0$, then the integral equation is used to get a better value of $k \cot \eta_1$. Thus by iteration we get better values of η and wavefunctions. This method converges to the correct $u(r)$ very rapidly if $u_0(r)$ is properly chosen.

The variational principle for bound states gives an upper bound for the energy of the ground state of the system; for a scattering system the value lies very close to $k \cot \eta_{\ell}$ but the sign of the error is not in general known. However, Schwinger's method does give a variational bound to $k \cot \eta$.^{9a}

Sugar and Blankenbecler^{31a} have based their proof on general non-local potentials. They have shown that in the case of purely repulsive potentials, Schwinger's method gives an upper bound for η and for purely attractive potentials, it gives a lower bound to η . No conclusions can be reached if V is not of one sign for all r . The results have also been applied to multichannel scattering.

Coulomb Field:

When the potential at large distances has a Coulomb behaviour i.e.

$$U(r) \sim \frac{C}{r}$$

then the asymptotic wavefunction is

$$u^C(r) \sim \sin(kr - \alpha \log 2kr + \eta + \sigma) \quad 35$$

where $\alpha = \frac{C}{2k}$, η is the phase shift due to the Coulomb field and σ that due to any modifications of the field that might occur. In this case the variational principle gives

$$\delta I = -k\delta(\eta + \sigma) \quad 36$$

and for the rest the same procedure follows.

Born Approximation:

In eq. 33, using the free particle wavefunction, the first term gives

$$[k \tan \eta]_{B1} = \int_0^{\infty} U(r) u^2(r) dr$$

which is the first Born approximation. The second term in the numerator gives the second Born approximation.

$$[k \tan \eta]_{B2} = - \int_0^{\infty} \int_0^{\infty} U(r) u(r) G(r, r') U(r') u(r') dr dr' .$$

To second Born approximation

$$[k \tan \eta]^{B2} = [k \tan \eta]_{B1} + [k \tan \eta]_{B2}$$

Thus to calculate lower order terms, Schwinger's method is the most appropriate to use for evaluating the stationary value of any quantity.

e. Variational Principle for Scattering Amplitude

In this section the stationary property of the scattering amplitude will be examined. The general solution for the Schrödinger equation

$$\{\nabla^2 + k^2 - U(\vec{r})\} \Psi(\vec{r}) = 0$$

is given by

$$\Psi(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} - \frac{1}{4\pi} \int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} U(\vec{r}') \Psi(\vec{r}') d\vec{r}' . \quad 37$$

For any large r , the asymptotic behaviour of Ψ is given by eq. I-72

$$\Psi(\vec{r}) \sim e^{i\vec{k} \cdot \vec{r}} + \frac{e^{ikr}}{r} f(\theta, \phi) . \quad 38$$

For large r we have

$$k|\vec{r}-\vec{r}'| \sim kr - \vec{k}_s \cdot \vec{r}', \quad 39$$

where \vec{k}_s has the magnitude of k and direction of the scattered wave. Substitute eq. 39 in 37, and then compare equations 37 and 38, to get the scattering amplitude as

$$f(\theta, \phi) = -\frac{1}{4\pi} \int e^{-i\vec{k}_s \cdot \vec{r}'} U(\vec{r}) \Psi(\vec{r}') d\vec{r}'. \quad 40$$

Since (θ, ϕ) is the direction of scattered wave with respect to the incident wave, we change our notation to

$$f(\theta, \phi) \equiv f(\vec{k}_s, \vec{k}).$$

The adjoint of Ψ is defined as

$$\tilde{\Psi} = e^{-i\vec{k}_s \cdot \vec{r}} - \frac{1}{4\pi} \int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} U(\vec{r}) \Psi(\vec{r}') d\vec{r}'. \quad 41$$

This means that the plane wave is incident in the direction opposite to that of the scattered wave.

Multiply eq. 37 by $\tilde{\Psi}U(\vec{r})$ and integrate, we get

$$\begin{aligned} \int \tilde{\Psi}(\vec{r}) U(\vec{r}) \Psi(\vec{r}) d\vec{r} &= \int \tilde{\Psi}(\vec{r}) U(\vec{r}) e^{i\vec{k} \cdot \vec{r}} d\vec{r} \\ &\quad - \frac{1}{4\pi} \int \int \tilde{\Psi}(\vec{r}) U(\vec{r}) \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} U(\vec{r}') \Psi(\vec{r}') d\vec{r} d\vec{r}'. \end{aligned}$$

Rearranging the terms and making use of equation 40

we obtain

$$f(\vec{k}_s, \vec{k}) = - \frac{\frac{1}{4\pi} \int \tilde{\Psi}(\vec{r}) U(\vec{r}) e^{i\vec{k} \cdot \vec{r}} d\vec{r} \int e^{-i\vec{k}_s \cdot \vec{r}'} U(\vec{r}') \Psi(\vec{r}') d\vec{r}'}{\int \tilde{\Psi}(\vec{r}) U(\vec{r}) \Psi(\vec{r}) d\vec{r} + \frac{1}{4\pi} \int \int \tilde{\Psi}(\vec{r}) U(\vec{r}) \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} U(\vec{r}') \Psi(\vec{r}') d\vec{r} d\vec{r}'} \quad 42$$

which gives the variational principle for the scattering amplitude. It can be verified from eq. 42 that

$$f(\vec{k}_s, \vec{k}) = f(-\vec{k}_s, -\vec{k}) \quad 43$$

which is the reciprocity theorem. We can show that if $f(\vec{k}_s, \vec{k})$ is stationary, then equations 37 and 41 are satisfied or vice versa.

Comments:

The various methods discussed have been shown to give the same results. The alternative procedures differ simply in their effectiveness in keeping the second and higher order terms small. Makinson and Turner^{15a} have shown that Kohn's condition can sometimes give better and sometimes worse values of η_ℓ than those given by Hulthén's. There is no way of knowing whether it is better or worse; it just depends on the trial wavefunction chosen. Hulthén's method gives more consistent results.

Kato^{9a} has shown that Schwinger's method always gives a larger (smaller) value of $k \cot \eta$ than does Hulthén's if $V(r) \geq 0$ ($V(r) \leq 0$) everywhere. Schwinger's method has

been shown to be the most elegant one in scattering problems for lower order variational calculations. But for higher order it becomes difficult to calculate the term involving the Green's function. In such cases Hulthén's method has been found to be the most suitable one.

All the above methods have been worked out in coordinate space which are, generally, applicable to simple collision problems. When disintegrations are involved, it is quite difficult to estimate the complicated asymptotic form of the wavefunction. However, it was shown by Dirac and Heisenberg that the asymptotic behaviour in coordinate space reflects itself by singularities in momentum space. Kohn^{12a} worked on a variational principle in momentum space and has given the stationary expressions for both Kohn-Hulthén and Schwinger types of $\tan\eta$.

Makinson and Turner^{15a} have compared variational and perturbation methods and have shown that these two methods are virtually the same; the second order perturbation and the expressions stationary to second order can be determined in the same manner.

f. Variational Principle Applied to Time Dependent Theory

The stationary properties of the operators S , T , K will be brought out by seeking different variational functions for these quantities.

Consider the functional defined by

$$S[U_-^\dagger, U_+] = U_+(\infty) - \int_{-\infty}^{+\infty} U_-^\dagger(t) \left\{ \frac{\partial}{\partial t} + \frac{i}{\hbar} H_I(t) \right\} U_+(t) dt \quad 44$$

with the restrictions $U_+(-\infty) = 1$, $U_-(+\infty) = 1$.

The change in $S[U_-^\dagger, U_+]$ due to small independent variations in U_+ and U_- is given, after partial integration, by

$$\begin{aligned} \delta S[U_-^\dagger, U_+] = & - \int_{-\infty}^{+\infty} \delta U_-^\dagger(t) \left\{ \frac{\partial}{\partial t} + \frac{i}{\hbar} H_I(t) \right\} U_+(t) dt \\ & + \int_{-\infty}^{+\infty} \left[\left(\frac{\partial}{\partial t} + \frac{i}{\hbar} H_I(t) \right) U_-(t) \right]^\dagger \delta U_+(t) dt . \end{aligned} \quad 45$$

Therefore, $S[U_-^\dagger, U_+]$ is stationary if $U_+(t)$ and $U_-(t)$ are the solutions of the differential equations

$$i\hbar \frac{\partial}{\partial t} U_+(t) = H_I(t) U_+(t)$$

$$i\hbar \frac{\partial}{\partial t} U_-(t) = H_I(t) U_-(t)$$

and the stationary value of eq. 44 is just the scattering operator S . The variational expression in integral form can be written as

$$\begin{aligned} S[U_-^\dagger, U_+] = & 1 - \frac{i}{\hbar} \int_{-\infty}^{+\infty} \{ U_-^\dagger(t) H_I(t) + H_I(t) U_+(t) \} dt \\ & + \frac{i}{\hbar} \int_{-\infty}^{+\infty} U_-^\dagger(t) H_I(t) U_+(t) dt \\ & + \left(\frac{i}{\hbar} \right)^2 \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} U_-^\dagger(t) H_I(t) \eta(t-t') H_I(t') U_+(t') dt dt' . \end{aligned}$$

Hence

$$\begin{aligned}
\delta S[U_-^\dagger, U_+] &= -\frac{i}{\hbar} \int_{-\infty}^{+\infty} \{ \delta U_-^\dagger(t) H_I(t) + H_I(t) \delta U_+(t) \} dt \\
&+ \frac{i}{\hbar} \int_{-\infty}^{+\infty} \delta U_-^\dagger(t) H_I(t) U_+(t) dt + \frac{i}{\hbar} \int_{-\infty}^{+\infty} U_-^\dagger(t) H_I(t) \delta U_+(t) dt \\
&+ \left(\frac{i}{\hbar}\right)^2 \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \delta U_-^\dagger(t) H_I(t) \eta(t-t') H_I(t') U_+(t') dt dt' \\
&+ \left(\frac{i}{\hbar}\right)^2 \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} U_-^\dagger(t) H_I(t) \eta(t-t') H_I(t') \delta U_+(t') dt dt' \\
&= \frac{i}{\hbar} \int_{-\infty}^{+\infty} \delta U_-^\dagger(t) H_I(t) [-1 + U_+(t) \\
&+ \frac{i}{\hbar} \int_{-\infty}^{+\infty} \eta(t-t') H_I(t') U_+(t') dt'] dt \\
&+ \frac{i}{\hbar} \int_{-\infty}^{+\infty} [-1 + U_-(t) \\
&+ \frac{i}{\hbar} \int_{-\infty}^{+\infty} \eta(t'-t) U_-^\dagger(t') H_I(t') dt'] H_I(t) \delta U_+(t) dt \\
&= \frac{i}{\hbar} \int_{-\infty}^{+\infty} \delta U_-^\dagger(t) H_I(t) [U_+(t) - 1 \\
&+ \frac{i}{\hbar} \int_{-\infty}^{+\infty} \eta(t-t') H_I(t') U_+(t') dt'] dt \\
&+ \frac{i}{\hbar} \int_{-\infty}^{+\infty} [U_-(t) - 1 \\
&- \frac{i}{\hbar} \int_{-\infty}^{+\infty} \eta(t'-t) H_I(t') U_-^\dagger(t') dt']^\dagger H_I(t) \delta U_+(t) dt .
\end{aligned}$$

For S to be stationary we get the following two equations

$$U_+(t) = 1 - \frac{i}{\hbar} \int_{-\infty}^{+\infty} \eta(t-t') H_I(t') U_+(t') dt'$$

$$U_-(t) = 1 + \frac{i}{\hbar} \int_{-\infty}^{+\infty} \eta(t'-t) H_I(t') U_-(t') dt'$$

which are just the equations to be satisfied by $U_+(t)$ and $U_-(t)$ operators. Also the stationary value is the scattering operator S itself. Eq. 46 differs from eq.44 in that no restrictions have been imposed on U_+ and U_- and every integral contains the interaction H_I . If the same trial operators are chosen, then eq.46 gives better values than eq.44. For example, if we put $U_+(t) = U_-(t) = 1$ in equations 44 and 46 then, eq. 44 yields

$$S = 1 - \frac{i}{\hbar} \int_{-\infty}^{+\infty} H_I(t) dt$$

which is equivalent to the first Born approximation. Eq.46 yields

$$S = 1 - \frac{i}{\hbar} \int_{-\infty}^{+\infty} H_I(t) dt + \left(\frac{i}{\hbar}\right)^2 \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} H_I(t) \eta(t-t') H_I(t') dt dt'$$

which is the second Born approximation.

The disadvantage of these variational expressions 44 and 46 is that when approximations are substituted, the unitarity of S is violated. To overcome this difficulty we introduce the reaction operator K which is Hermitian. With this we can make the unitarity of S manifest, as will be obvious below.

We already have the relations from Chapter I, equations 29 and 33

$$V(t) = U_+(t) \frac{2}{1+S} = U_-(t) \frac{2}{1+S^{-1}}$$

$$S = \frac{V(\infty)}{V(-\infty)} = \frac{1 - \frac{1}{2} iK}{1 + \frac{1}{2} iK}.$$

The variational expression for K is given by

$$\begin{aligned} K[V(t), V^\dagger(t)] &= \frac{1}{\hbar} \int_{-\infty}^{+\infty} [H_I(t)V(t) + V^\dagger(t)H_I(t)]dt \\ &\quad - \frac{1}{\hbar} \int_{-\infty}^{+\infty} V^\dagger(t)H_I(t)V(t)dt \\ &\quad - \frac{i}{2\hbar^2} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} V^\dagger(t)H_I(t)\epsilon(t-t')H_I(t')V(t')dt dt' \end{aligned}$$

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which is Hermitian for arbitrary $V(t)$ as can be verified easily. Vary $V(t)$ and $V^\dagger(t)$ by $\delta V(t)$ and $\delta V^\dagger(t)$, then we get

$$\begin{aligned} \delta K[V, V^\dagger] &= -\frac{1}{\hbar} \int_{-\infty}^{+\infty} \delta V^\dagger(t)H_I(t)[V(t) - 1 \\ &\quad + \frac{i}{2\hbar} \int_{-\infty}^{+\infty} \epsilon(t-t')H_I(t')V(t')dt']dt \\ &\quad - \frac{1}{\hbar} \int_{-\infty}^{+\infty} [V(t) - 1 + \frac{i}{2\hbar} \int_{-\infty}^{+\infty} \epsilon(t-t')H_I(t')V(t')dt'] \\ &\quad \times H_I(t)\delta V(t)dt \end{aligned}$$

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which is zero if

$$V(t) = 1 - \frac{i}{2\hbar} \int_{-\infty}^{+\infty} \varepsilon(t-t') H_I(t') V(t') dt'.$$

The stationary value is

$$K = \frac{1}{\hbar} \int_{-\infty}^{+\infty} H_I(t) V(t) dt.$$

The variational expression for K in the differential form is written as

$$\begin{aligned} K[V, V^\dagger] = & -\frac{i}{2} \int_{-\infty}^{+\infty} [V^\dagger(t) \frac{\partial V(t)}{\partial t} - \frac{\partial V^\dagger(t)}{\partial t} V(t)] dt \\ & + \frac{1}{\hbar} \int_{-\infty}^{+\infty} V^\dagger(t) H_I(t) V(t) dt \\ & + \frac{i}{2} [\{V(\infty) - V(-\infty)\} - \{V^\dagger(\infty) - V^\dagger(-\infty)\}]. \quad 50 \end{aligned}$$

Expression 50 is Hermitian for any $V(t)$ as required. The change in K is given by

$$\begin{aligned} \delta K[V, V^\dagger] = & -\frac{1}{\hbar} \int_{-\infty}^{+\infty} [\delta V^\dagger(t) \{i\hbar \frac{\partial}{\partial t} - H_I(t)\} V(t) \\ & + \{(i\hbar \frac{\partial}{\partial t} - H_I(t)) V(t)\}^\dagger \delta V(t)] dt \\ & - \frac{i}{2} [\{V^\dagger(\infty) + V^\dagger(-\infty)\} \delta(V(\infty) + V(-\infty)) \\ & + (\frac{V^\dagger(\infty) + V^\dagger(-\infty)}{2} - 1) \delta\{V(\infty) - V(-\infty)\} \\ & - \delta(\frac{V^\dagger(\infty) + V^\dagger(-\infty)}{2}) \{V(\infty) - V(-\infty)\} \\ & - \delta\{V^\dagger(\infty) - V^\dagger(-\infty)\} (\frac{V(\infty) + V(-\infty)}{2})] \end{aligned}$$

$$\delta K[V, V^\dagger] = 0$$

if

$$[i\hbar \frac{\partial}{\partial t} - H_I(t)] V(t) = 0$$

and the stationary value is K itself.

The Lippmann-Schwinger equation can be derived from the variational expression for T_{ba} . From equation 44 and equation 18 (Chap. I) we get

$$\begin{aligned} T_{ba}[\psi_b, \psi_a] = & -\frac{i}{\hbar} \int_{-\infty}^{+\infty} dt [\langle e^{i(E_a - H_0)\frac{t}{\hbar}} U_-(t) \phi_b | H_I | \phi_a \rangle \\ & + \langle \phi_b | H_I | e^{i(E_b - H_0)\frac{t}{\hbar}} U_+(t) \phi_a \rangle] \\ & + \frac{i}{\hbar} \int_{-\infty}^{+\infty} dt [\langle e^{-iH_0\frac{t}{\hbar}} U_-(t) \phi_b | H_I | e^{-iH_0\frac{t}{\hbar}} U_+(t) \phi_a \rangle] \\ & + \left(\frac{i}{\hbar}\right)^2 \int_{-\infty}^{+\infty} dt \int_{-\infty}^{+\infty} dt' \langle e^{-iH_0\frac{t}{\hbar}} U_-(t) \phi_b | H_I e^{-iH_0\frac{(t-t')}{\hbar}} \times \\ & H_I | e^{-iH_0\frac{t'}{\hbar}} U_+(t') \phi_a \rangle . \end{aligned} \quad 51$$

In the interaction picture $U_+(t)|\phi_a\rangle$ is an eigenstate of H at any time t which has evolved from $|\psi(-\infty)\rangle = |\phi_a\rangle$; in Schrödinger picture. Therefore, $e^{-iH_0\frac{t}{\hbar}} U_+(t)|\phi_a\rangle$ is the eigenstate of H (eq. I-2). If ψ_a^+ is the stationary eigenstate of H with eigenvalue E_a , then $e^{-iH_0\frac{t}{\hbar}} |\psi_a\rangle$ is the eigenstate of H in Schrödinger picture. Hence, we can write

$$e^{-iH_0 \frac{t}{\hbar}} U_+(t) |\phi_a\rangle = e^{-iE_a \frac{t}{\hbar}} |\psi_a^+\rangle \quad . \quad 52$$

Integrate eq. 51; (using eq. 52) we get

$$\begin{aligned} T_{ba}[\psi_b, \psi_a] = & -2\pi i \delta(E_b - E_a) [\langle \psi_b^- | H_I | \phi_a \rangle + \langle \phi_b | H_I | \psi_a^+ \rangle \\ & - \langle \psi_b^- | H_I | \psi_a^+ \rangle + \langle \psi_b^- | H_I \frac{1}{E - H_0 + i\epsilon} H_I | \psi_a^+ \rangle] \end{aligned}$$

where E is the common energy of states a and b . The variation in T_{ba} is given by

$$\begin{aligned} \delta T_{ba}[\psi_b, \psi_a] = & \langle \delta \psi_b^- | H_I | (\phi_a + \frac{1}{E - H_0 + i\epsilon} H_I \psi_a^+ - \psi_a^+) \rangle \\ & + \langle (\phi_b + \frac{1}{E - H_0 - i\epsilon} H_I \psi_b^- - \psi_b^-) | H_I | \delta \psi_a^+ \rangle. \quad 53 \end{aligned}$$

For arbitrary variations $\delta \psi_b$ and $\delta \psi_a$, $\delta T_{ba} = 0$ gives

$$|\psi_a^+\rangle = |\phi_a\rangle + \frac{1}{E - H_0 + i\epsilon} H_I |\psi_a^+\rangle$$

$$|\psi_a^-\rangle = |\phi_a\rangle + \frac{1}{E - H_0 - i\epsilon} H_I |\psi_a^-\rangle$$

which are the Lippmann-Schwinger equations. The stationary value of eq. 51 is T_{ba} , as can be seen from the following expression:

$$\begin{aligned} \langle \psi_b^- | H_I | \psi_a^+ \rangle - \langle \psi_b^- | H_I \frac{1}{E - H_0 + i\epsilon} H_I | \psi_a^+ \rangle &= \langle \psi_b^- | H_I | \phi_a \rangle \\ &= \langle \phi_b | H_I | \psi_a^+ \rangle \quad . \end{aligned}$$

The variational principle in terms of the scattering operator formalism is more general than that in terms of the phase shifts. Moses^{16a} has worked out the Kohn-Hulthén method in this formalism and explains how to get better values of T_{ba} and ψ^{\pm} by iteration.

CHAPTER IV

APPLICATIONS OF VARIATIONAL PRINCIPLE

a. Effective Range Theory

The internuclear forces are quite complicated and still not well understood. To explain the main features of nucleon-nucleon scattering at low energies, a few basic assumptions can be made and later, the other corrections brought in. We assume that the internuclear forces are strong, short ranged and conservative. Furthermore, they are taken to be spin-independent and central: no detailed law of force is required. That amounts to saying that we shall be dealing with the overall effect of depth and range of the potential and not bother about the shape. For example, if the range is small, the potential depth has to be large in order that bound states can exist. Thus the results depend on the combined effect of depth and range and not on each parameter separately.

If the energy of the incident nucleon is less than ~ 10 Mev., its wavelength is long enough so that only S-wave ($l = 0$) scattering takes place. However, it is assumed that the energy of the incident nucleon is much greater than the binding energy of the target nucleon so that the latter is taken to be essentially a free particle. At these low energies, the scattering amplitude and total scattering cross section can be written as

$$f(\theta) = \frac{1}{2ik} [e^{2i\eta_0} - 1] \quad 1$$

$$\sigma = \frac{4\pi}{k^2} \sin^2 \eta_0 . \quad 2$$

At $k = 0$, $\ell = 0$, there are other convenient parameters connected with scattering rather than the phase shifts. Schwinger expressed the phase shifts in terms of these parameters by a variational technique. Later, Bethe gave a different method. Before giving Schwinger's method, we shall familiarise ourselves with these parameters.

The radial wavefunction $u_0(k, r)$ for $\ell = 0$ satisfies the equation (suppressing index 0 throughout IVa),

$$\frac{d^2}{dr^2} u(k, r) + k^2 u(k, r) - U(r)u(k, r) = 0 . \quad 3$$

The asymptotic form of the solution of 3 is $A \sin(kr + \eta)$.

It can be normalised so that

$$u(k, r) \xrightarrow{r \rightarrow \infty} \frac{\sin(kr + \eta)}{\sin \eta} \equiv v(k, r) . \quad 4a$$

This defines the function $v(k, r)$, which coincides with $u(k, r)$ in asymptotic regions and is unity at $r = 0$.

Obviously, $v(k, r)$ satisfies the equation

$$\frac{d^2 v(k, r)}{dr^2} + k^2 v(k, r) = 0 . \quad 5a$$

Hence, the solution for $k = 0$ is

$$v(0, r) = c(r - a) . \quad 6a$$

To fix the constant c , expand $v(k,r)$ in eq.4a in powers of r :

$$v(k,r) \approx \frac{1}{\sin\eta} (\sin\eta + kr \cos\eta - \frac{k^2 r^2}{2} \sin\eta + \dots) . \quad 4b$$

Comparing equations 6a and 4b we get

$$c = -\frac{1}{a} \quad 7a$$

and

$$\lim_{k \rightarrow 0} k \cot\eta = -\frac{1}{a} . \quad 7b$$

The quantity a is called Fermi's scattering length. Eq.7b gives

$$\tan\eta = -ka .$$

Substitute this value in eq. 2, for $k = 0$ to get for the total scattering cross section

$$\sigma = 4\pi a^2 .$$

This is identical to the scattering cross section from an impenetrable sphere of radius a . Equation 6a can be written as

$$v(0,k) = 1 - \frac{r}{a} \equiv 1 - \alpha r \quad 6b$$

where the constant α for $\frac{1}{a}$ has been introduced for later convenience. The other parameter introduced at low energies is the 'effective range' defined by

$$r_0 = 2 \int_0^\infty \{v^2(0,r) - u^2(0,r)\} dr . \quad 8$$

Finally, in terms of these two quantities, the 'shape independent' formula derived is

$$k \cot \eta = -\frac{1}{a} + k^2 \int_0^\infty \{v^2(0,r) - u^2(0,r)\} dr . \quad 9$$

The second term on the R.H.S. of eq. 9 is called the 'range correction'. Before this term was introduced, previous workers had assumed zero range and the results were not satisfactory. The name 'shape independent' comes from the fact that a very general form of potential is assumed for deriving eq. 9. Two different well shapes can give approximately the same values of a and r_0 as long as the higher order terms in k can be kept negligible.

Now we derive formula 9 from Schwinger's variational principle. From eq. 30, Chap. III we have

$$k \cot \eta = - \frac{\int_0^\infty U(r) \{u(r)\}^2 dr + \int_0^\infty U(r) u(r) dr \int_0^\infty G(r, r') U(r') u(r') dr'}{\left[\int_0^\infty r j_0(kr) U(r) dr \right]^2} .$$

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Choose the trial wavefunction at a fixed energy. Schwinger replaces $u(r)$ in eq. 10 by a zero energy wavefunction which satisfies

$$\left[\frac{d^2}{dr^2} - U(r) \right] u(0,r) = 0 \quad r \leq b \quad 5b$$

and which has the solution 6 for $r > b$. In general, for $k^2 \neq 0$, the solution outside is not a straight line but has

the form 4a. This choice of $u(0,r)$ as a trial function therefore seems to be very poor. However, we are not concerned with the solutions outside because $u(r)$ occurs in combination as $U(r)u(r)$. Inside, the solutions of equations 3 and 5b differ by the order of k^2 which is very small at low energies. But the solutions outside and inside with the same k are related; therefore, we would be justified in taking the trial wavefunction $u(0,r)$ suggested by its outside behaviour.

Therefore we define the function $g(r)$ by

$$u(0,r) = 1 - \alpha r - g(r) \quad \text{for all } r . \quad 11$$

The boundary conditions on $g(r)$ are:

$$u(0,0) = 0, \quad \text{implying} \quad g(0) = 1 .$$

Eq. 7 gives $g(r) = 0$ for $r > b$. Equations 5b and 11 give

$$\frac{d^2 u(0,r)}{dr^2} = - \frac{d^2 g(r)}{dr^2} = U(r)u(0,r) . \quad 12$$

In order to calculate the expression in eq. 10 with this trial wavefunction, first consider the integral

$$J(r) \equiv - \int_0^{\infty} G(r,r') U(r') u(0,r') dr' . \quad 13a$$

Substitute equation 12 in equation 13a and integrate twice by parts, to get

$$J(r) = \left[G(r, r') \frac{dg}{dr'} - \frac{dG(r, r')}{dr'} g(r') \right]_{r'=0}^{r'=\infty} \\ + \int_0^{\infty} g(r') \frac{d^2 G}{dr'^2}(r, r') dr' .$$

Using the values $G(r, 0) \sim 0$, $\left. \frac{dG}{dr'} \right|_{r'=0} \sim \cos kr$ and $\left. \frac{dg}{dr'} \right|_{r' \rightarrow \infty} = 0$ and also substituting for $\frac{d^2 G}{dr'^2}$, we get

$$J(r) = \cos(kr) - g(r) - k^2 \int_0^{\infty} G(r, r') g(r') dr' . \quad 13b$$

The numerator, N , of eq. 10 can be written then, with the help of equations 12 and 13b, as

$$N = \int_0^{\infty} \frac{d^2 g}{dr^2} [u(0, r) - J(r)] dr \\ \approx -\alpha + k^2 \int_0^{\infty} [2g(r) \cos kr - g^2(r)] dr . \quad 14$$

Terms involving $O(k^4)$ have been dropped in writing down eq. 14. The denominator of eq. 10 can be written as

$$D^{\frac{1}{2}} = - \int_0^{\infty} \frac{1}{k} \sin kr U(r) u(r) dr \\ = \frac{1}{k} \int_0^{\infty} \sin kr \frac{d^2 g}{dr^2} dr \\ \sim 1 - k^2 \int_0^{\infty} r g(r) dr \quad 15$$

since $j_0(kr) = \frac{\sin kr}{kr}$.

Keeping terms up to the order of k^2 only we get

$$D^{-1} \sim 1 + 2k^2 \int_0^{\infty} r g(r) dr . \quad 16$$

Combining equations 14 and 16 we get

$$k \cot \eta = ND^{-1} \\ \approx -\alpha + \frac{1}{2} r_0 k^2 + (\text{higher order terms}) \quad 17$$

where the effective range is given by

$$r_0 = 2 \int_0^{\infty} [(1-\alpha r)^2 - u^2(0,r)] dr \quad 18$$

which is the same as in eq. 8.

A modified 'effective range theory' has been given by O'Malley et al for long range potentials and higher angular momenta.^{26a}

These low energy parameters a and r_0 can help to determine the rate of photo transition and Bremsstrahlung. The bound state problem can similarly be analysed by using two parameters.

The above simplified argument explains only the simple elastic scattering. To explain the larger cross sections observed than those calculated above, spins had to be included. The scattering lengths and effective ranges are different for different spin combinations.

To include the observed quadrupole moment of the deuteron, non-central forces are used. In fact, more and more complications like parity, Coulomb interaction, etc. had to come in to explain the observed data. The effective range theory has also been further extended to include higher angular momenta.

b. Upper Bounds to Scattering Lengths

As is well known in the calculation of energy for the ground state of a system, it is possible to get upper bounds for the energy, and it is not straightforward and easy to get it for the excited states. However, in the variational method for scattering problems one can get the upper bound for scattering lengths, even when bound states exist.

We shall consider a system where no bound states exist because in section IVa we have defined the scattering length for $E > 0$ only. However, the results can be generalised to bound states also.^{B6,B5,B13}

If H is the Hamiltonian of the system, then for any square integrable function χ ,

$$\int \chi H \chi \geq 0 \quad .$$

We have defined the operator L , III-8; for $k = 0$ and $\ell = 0$ we have

$$L = \frac{d^2}{dr^2} - U(r) .$$

Since $H \propto -L$, we have

$$\int \chi L \chi \leq 0 . \quad 19$$

Instead of the asymptotic expression given by eq. 7, Kohn uses the asymptotic condition

$$u(r) \sim a - r \quad 20$$

where a is the scattering length. This expression gives a result directly in terms of a , whereas if expression 7 is used, the result is in terms of inverse scattering length.

The trial wavefunction at low energies should satisfy the boundary conditions

$$u_T(0) = 0$$

$$u_T(r) \sim a_T - r \quad \text{for large } r . \quad 21$$

$u_T(r)$ is the trial function with a_T as the trial value for the scattering length. Put

$$\omega(r) = u_T(r) - u(r)$$

where $u(r)$ is the exact wavefunction such that $Lu(r) = 0$. Then the functional I_T can be calculated as follows:

$$\begin{aligned}
I &= \int_0^{\infty} u_T L u_T \\
&= \int_0^{\infty} (\omega+u) \frac{d^2}{dr^2} (\omega+u) - \int_0^{\infty} (\omega+u) U(r) (\omega+u) dr \\
&= u(\infty) \left. \frac{d\omega}{dr} \right|_{\infty} - \omega(\infty) \left. \frac{du}{dr} \right|_{\infty} + \int_0^{\infty} \omega L \omega dr .
\end{aligned}$$

$$\int_0^{\infty} u_T L u_T dr = (a_T - a) + \int_0^{\infty} \omega L \omega dr$$

$$\text{or} \quad a = a_T + \int_0^{\infty} \omega L \omega dr - \int_0^{\infty} u_T L u_T dr .$$

To insure the convergence of the integrations we take the Abel limit. Then

$$\int_0^{\infty} \omega L \omega \leq 0 .$$

Consequently we get

$$a \leq a_T - I_T \tag{21}$$

which provides an upper bound for the scattering length. The right hand expression can be calculated from Kohn's, Hulthén's or Tamm's variational methods.

c. Monotonic Property of Phase Shifts

Consider two scattering potentials $V_a(r)$ and $V_b(r)$, both positive. Kato's variational expression will be used to prove that for two partial waves of same energy, k , and

angular momentum, ℓ , the phase shifts satisfy the relation

$$\eta_a \leq \eta_b \quad \text{if} \quad V_a(r) \geq V_b(r) \quad \text{for all } r .$$

Assume $V_a(r) - V_b(r)$ to be an infinitesimal positive quantity and let the radial wave functions be $u_a(r)$ and $u_b(r)$ respectively. From Kato's expression eq. III, 22b

$$k\alpha = k\zeta - \int_0^\infty vLvdr \quad 22$$

we get

$$k \cot(\eta_a - \theta) = k \cot(\eta_b - \theta) - \int_0^\infty u_b L u_b dr .$$

For the same k and ℓ and from the equations

$$L_a u_a = 0 , \quad L_b u_b = 0$$

we get

$$L_a u_b = (U_b - U_a)u_b . \quad 23$$

Substituting u_b for v and $L_a u_b$ for Lv in eq. 22 we get

$$k \cot(\eta_a - \theta) = k \cot(\eta_b - \theta) + \int_0^\infty (U_a - U_b)u_b^2 dr .$$

Since the integral on R.H.S. is positive definite we get

$$\cot(\eta_a - \theta) - \cot(\eta_b - \theta) \geq 0 .$$

Since θ is at our disposal, choose $\theta = \frac{\pi}{2}$; we get

$$\tan \eta_b \geq \tan \eta_a .$$

Since $(U_a - U_b)$ is very small, and U_a and U_b have the same sign it follows that both η_a and η_b have the same sign. Therefore we get

$$\eta_b \geq \eta_a \quad . \quad 24$$

We can add up the infinitesimals and show that the result is true for finite potential differences also. It follows from this result that phase shifts are positive for $V(r) \leq 0$ for all r and negative if $V(r) \geq 0$ for all r .

d. Application to the Determination of Wavefunctions and Phase Shifts

Before variational methods were developed, there were no sufficiently reliable methods to include effects like exchange forces and polarisation for calculating phase shifts. However, variational techniques have successfully been applied to scattering where these effects have been taken into account. The first problem to be studied was the scattering of an electron by a hydrogen atom by Huang.^{5a} He made an allowance for polarisation but not exchange. Great improvement was shown by Massey and Moiseiwitsch^{13a} by including both these effects. Checks on the validity of the variational technique have been made by comparing the results with those of numerical integration.

The usual procedure consists of the following steps: From the experimental cross sections, phase shifts

are obtained. To explain the observed data, trial wavefunctions are assumed from which the variational parameters are calculated, these will give the theoretical phase shifts. The theoretical and experimental results are then compared. If the results are far apart, then the assumptions and approximations for choosing the trial wavefunctions are modified till we get consistent results.

As an example, consider the elastic scattering of an electron by a hydrogen atom as treated by Massey and Moiseiwitsch.^{13a} For the one body approximation i.e. when the trial wavefunction was unsymmetric and polarisation was neglected, the results were not very sensitive to the form of trial wavefunction, as long as it satisfied the correct boundary conditions. Let r_1 be the coordinate of the electron in the atom with respect to the nucleus, r_2 that of the incident electron, and r_{12} the distance between the two electrons. The one-body approximation wavefunction was

$$\begin{aligned}
 (a) \quad \psi_t &= \frac{1}{r^2} e^{-r_1} \{ \sin kr_2 + (\alpha + \beta e^{-r_2})(1 - e^{-r_2}) \cos kr_2 \} \\
 &\equiv \psi_t^{(1)}(r_1, r_2) .
 \end{aligned}$$

It does not depend on the relative co-ordinates of the two electrons. When this is included, it is called the polarisation approximation and the trial wavefunction chosen was

$$\begin{aligned}
 (b) \quad \psi_t &= \frac{1}{r^2} e^{-r_1} \{ \sin kr_2 + [\alpha + (\beta + \gamma r_{12}) e^{-r_2}] (1 - e^{-r_2}) \cos kr_2 \} \\
 &\equiv \psi_t^{(2)}(r_1, r_2, r_{12}) .
 \end{aligned}$$

The wavefunctions (a) and (b) are unsymmetrical. The exchange approximation takes care of the symmetry of the trial wavefunction, which was chosen as

$$(c) \quad \psi_t = \psi_t^{(1)}(r_1, r_2) \pm \psi_t^{(1)}(r_2, r_1) .$$

Finally, the trial wavefunction taking care of both, the exchange and polarisation approximations, is

$$(d) \quad \psi_t = \psi_t^{(2)}(r_1, r_2, r_{12}) \pm \psi_t^{(2)}(r_2, r_1, r_{12}) .$$

For the one-body approximation, phase shifts have been found to be quite identical with those from numerical integration.

For the polarisation approximation, the agreement is good at certain energies only. Also, it has been shown that the inclusion of parameters β and γ does not affect the results very much.

In case (d) the observation is that the polarisation effect contributes very little when the exchange effect is included, but otherwise it is very important by itself.

The trial wavefunction selected is such that it satisfies the correct asymptotic conditions. However, it is exact if, in addition to the asymptotic conditions, it satisfies the differential equation.

In this paper, Massey and Moiseiwitsch have shown that the symmetric wavefunction does not satisfy the differential equation and the phase shifts given are less accurate than those given by the exact wavefunction. On the other hand, the antisymmetric function gives very good values of phase shifts, but still does not satisfy the differential equation. Therefore, to avoid tedious calculations and not gain much in the final results, it is better to work with simple trial functions with correct asymptotic forms.

Extensive studies in the case of inelastic scattering of electrons by hydrogen, positrons by hydrogen, neutrons by deuterons, etc. have been done. Similar techniques have also been widely applied to the formal theory of scattering.

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